CONSISTENCY ANALYSIS OF BILEVEL DATA-DRIVEN LEARNING IN INVERSE PROBLEMS

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Abstract. One fundamental problem when solving inverse problems is how to find regularization parameters. This article considers solving this problem using data-driven bilevel optimization, i.e. we consider the adaptive learning of the regularization parameter from data by means of optimization. This approach can be interpreted as solving an empirical risk minimization problem, and we analyze its performance in the large data sample size limit for general nonlinear problems. To reduce the associated computational cost, online numerical schemes are derived using the stochastic gradient method. We prove convergence of these numerical schemes under suitable assumptions on the forward problem. Numerical experiments are presented illustrating the theoretical results and demonstrating the applicability and efficiency of the proposed approaches for various linear and nonlinear inverse problems, including Darcy flow, the eikonal equation, and an image denoising example.

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1. Introduction

Data-driven modeling seeks to improve model accuracy and predictability by exploiting informations from existing data. It has lead to a wide range of successes in deep learning, reinforcement learning, natural language processing and others [26, 28, 47]. This article is interested in its applications when solving inverse problem. Mathematically speaking, when solving an inverse problems, we try to recover a \( u \in \mathcal{U} \) from perturbed data \( y \in \mathcal{Y} \) where the relationship is given as

\[
(1.1) \quad y = \mathcal{G}(u) + \eta.
\]

In (1.1), \( \eta \sim \mathcal{N}(0, \Gamma) \) is an additive Gaussian noise and \( \mathcal{G} : \mathcal{U} \to \mathcal{Y} \) is the mapping from the parameter space \( \mathcal{U} \) to the observation space \( \mathcal{Y} \). Here, \( \mathcal{U} \) and \( \mathcal{Y} \) denote possibly infinite dimensional Banach spaces. Solutions to inverse problems have been well-studied through the use of variational and optimization methods which are well-documented in the following texts [24, 49].

Regularization is an important aspect of the numerical treatment of inverse problems. It helps overcoming the ill-posedness problem in theory and the overfitting phenomenon in practice. It can also be interpreted as a form of a-priori knowledge in the Bayesian approach [48, 32]. To implement regularization on (1.1), we estimate the unknown parameters by minimizing a regularized loss function, i.e. we consider

\[
(1.2) \quad u_* := \arg \min_{u \in \mathcal{U}} \mathcal{L}_{\mathcal{Y}}(\mathcal{G}(u), y) + \mathcal{S}_\lambda(u), \quad \lambda \in \mathbb{R}^+,
\]

where \( \mathcal{L}_{\mathcal{Y}} : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}^+ \) is some metric in \( \mathcal{Y} \) and \( \mathcal{S}_\lambda : \mathcal{U} \to \mathbb{R}^+ \) is a regularization function with regularization parameter \( \lambda > 0 \). A common choice is Tikhonov regularization [50] which can be included in (1.2) through the penalty term \( \mathcal{S}_\lambda(u) = \frac{\lambda}{2} \| u \|^2_{\mathcal{U}} \). The choice of norm \( \| \cdot \|_{\mathcal{U}} \) often models prior information on the unknown
parameter. Other common forms include $L_1$ and total variation regularization, which are particularly useful for imaging purposes [4, 24, 37].

In (1.2), the parameter $\lambda$ balances the influence of the data and the a-priori knowledge via the regularization. While expert knowledge can often provide a rough range of $\lambda$, the exact value, i.e. the $\lambda$ leading to the best estimation of the unknown parameter $u$, is often difficult to determine. However, the parameter $\lambda$ strongly influences the accuracy of the estimate and has to be properly chosen. Bilevel optimization is one way to resolve this issue [17, 21, 45, 49]. It seeks to learn the regularization parameter in a variational manner, and it can be viewed as a data-driven regularization [2]. To formulate this approach, we view unknown parameter $U \in \mathcal{U}$ and the data $Y \in \mathcal{Y}$ in the model (1.1) as a jointly distributed random variable with distribution $\mu(U, Y)$. To find the best possible regularization parameter of the model (1.1), the bilevel minimization seeks to solve

$$
\lambda_* = \arg \min_{\lambda > 0} F(\lambda), \quad F(\lambda) = \mathbb{E}_{\mu(U, Y)}[\mathcal{L}_U(u_{\lambda}(Y), U)], \quad \text{(upper level)}
$$

$$
u_{\lambda}(Y) := \arg \min_{u \in \mathcal{U}} \mathcal{L}_Y(G(u), Y) + S_{\lambda}(u), \quad \text{(lower level)}
$$

where $\mathcal{L}_U : \mathcal{U} \times \mathcal{U} \to \mathbb{R}_+$ is some metric in the parameter space $\mathcal{U}$. The upper level problem seeks to minimize the distance between the unknown parameter $U$ and the regularized solution corresponding to its data $Y$, which is computed through $u_{\lambda}(Y)$ in the lower level problem. To solve this (stochastic) bilevel optimization problem, we assume that we have access to training data, given through samples of $(U_i, Y_i) \sim \mu(U, Y)$, and the function $F$ in (1.3) can be approximated by its empirical Monte-Carlo approximation. The area of bilevel optimization has been applied to various methodologies for inverse problems. To motivate this we provide various examples of the application of bilevel optimization, in the setting describe by (1.3), to inverse problems and an overview of recent literature.

1.1. Motivating Examples.

1.1.1. Example 1 - PDE-constrained inverse problems. We first consider a inverse problem (1.1) with the lower level problem formulated by a partial differential equation (PDE):

$$
\arg \min_{u \in \mathcal{U}} \mathcal{L}_Y(O(p), y) + S_{\lambda}(u), \quad \text{s.t.} \ M(u, p) = 0,
$$

where $u \in \mathcal{U}$ denotes the unknown parameter and $p \in \mathcal{V}$ is the state. The function $M : \mathcal{U} \times \mathcal{V} \to \mathcal{W}$ describes an underlying ODE or PDE model. The operator $O : \mathcal{V} \to \mathbb{R}^K$ denotes the observation operator which maps the state $p$ to finite dimensional observations. The Darcy’s flow problem is one such example. In particular, $u$ describes a subsurface structure, $p$ is the corresponding pressure field, $M$ describes the Darcy’s law, and $O$ evaluate $p$ at different locations.

In order to formulate the corresponding bilevel problem (1.3), we assume that the forward model $M(u, p) = 0$ is well-posed, which means that for each $u \in \mathcal{U}$ there exists a unique $p \in \mathcal{V}$ such that $M(u, p) = 0 \in \mathcal{W}$. Hence, using the solution operator $G : \mathcal{U} \to \mathcal{V}$ s.t. $M(u, G(u)) = 0$, we can formulate the reduced problem of (1.4) by

$$
\arg \min_{u \in \mathcal{U}} \mathcal{L}_Y(G(u), y) + S_{\lambda}(u),
$$
where we have defined $G = \mathcal{O} \circ G$. Hence, given a training data set $(u^{(j)}, y^{(j)})$ we can also formulate the empirical bilevel minimization problem

$$\hat{\lambda}_n := \arg \min_{\lambda > 0} \frac{1}{n} \sum_{j=1}^{n} \| u^{(j)}(y^{(j)}) - u^{(j)} \|_2^2,$$

$$u^{(j)} := \arg \min_{u \in \mathcal{U}} L_Y(G(u), y^{(j)}) + S(u).$$

In terms of applications, many inverse problems arising in PDEs [3] are concerned with the recovery of an unknown which is heterogeneous. As a result it is very natural to model the unknown as a Gaussian random fields. Such models include Darcy flow, the Navier–Stokes model [30] and electrical impedance tomography [5, 32]. Physical constraints such as boundary, or initial conditions are required for modeling purposes.

Holler et al. [29] consider bilevel optimization for inverse problems in the setting of (1.4). They provide theory which suggests existence of solutions and formulate their problem as an optimal control problem. This is connected with the work of Kaltenbacher [33, 34] who provided a modified approach known as “all-at-once” inversion. These works have also been used in the context of deconvolution [13, 46].

1.1.2. Example 2 - Image & signal processing. Bilevel optimization is a popular solution choice for image processing problems [6, 35]. In these problems, one is interested in optimizing over an underlying image and particular areas/segments of that image. A common example of this includes image denoising which is to remove noise from an image. Another example is image deblurring where the image is commonly given as a convolution with a linear kernel $A$, i.e.

$$y = A \ast u + \eta,$$

where $\ast$ denotes the convolution of $A$ and $u$, commonly expressed as

$$A \ast u(x) = \int_{\mathbb{R}^d} A(x - \tau)u(\tau)d\tau.$$

This inverse problem is also known as deconvolution. The setting of (1.3) is common for deconvolution, where their loss functions are given as

$$\hat{\lambda}_n := \arg \min_{\lambda > 0} \frac{1}{n} \sum_{j=1}^{n} \| u^{(j)}(y^{(j)}) - u^{(j)} \|_2^2,$$

$$u^{(j)} := \arg \min_{u \in \mathcal{U}} L_Y(A \ast u, y^{(j)}) + \lambda \| Lu \|_2^2.$$

In (1.5), $L$ is a regularization matrix, and the upper level problem is taken as the minimization of the empirical loss function given by a training data set $(u^{(j)}, y^{(j)})$. Commonly $\lambda$ is taken to be either a weighted function between $L_Y$ and the penalty term, or it can be viewed as the noise within a system. Common choices of $L$ traditionally are $L = I$ or a first or second order operator, which can depend on the unknown or image of interest. Further detail on the choice of $L$ and $A$ are discussed in [6].

The work of De los Reyes, Schönlieb [9, 18, 19, 20] and coauthors considered the application of bilevel optimization to denoising and deblurring, where non-smooth regularization is used such as total variation and Bregman regularization. The latter forms of regularization are useful in imaging as they preserve non-smooth features, such as edges and straight lines.
1.2. Our contributions. In this article, we investigate two different approaches to solve bilevel optimization and their performance on inverse problems. Firstly we formulate the offline approach of bilevel optimization as an empirical risk minimization (ERM) problem. Analyzing the performance of the ERM solution is difficult, since the loss function is random and non-convex, so numerical solutions often can only find local minimums. We build a theoretical framework under these general settings. In particular, it provides convergence rate of the ERM solution when sample size goes to infinity. This framework is applied to linear inverse problems to understand the performance of bilevel optimization approach.

Secondly, we discuss how to implement stochastic gradient descent (SGD) methods on bilevel optimization. SGD is a popular optimization tool for empirical risk minimization because of its straightforward implementation and efficiency. The low computational costs are particularly appealing in the bilevel context as finding the lower-level solution is already time consuming. Besides exact SGD, we also consider SGD with central difference approximation. This can be useful for problems with complicated forward observation models. A general consistency analysis framework is formulated for both exact SGD and approximated SGD. We demonstrate how to apply this framework to linear inverse problems.

Various numerical results are presented highlighting and verifying the theory acquired. Our results are firstly presented on various partial differential equations both linear and nonlinear which include Darcy flow and the eikonal equation, as motivated through Example 1 in subsection 1.1.1. We also test our theory on an image denoising example which is discussed through Example 2 in subsection 1.1.2. In particular, we demonstrate numerically the statistical consistency result which includes the rate of convergence and we show the learned parameter $\lambda$ within each inverse problem experiment outperforms that with a fixed $\lambda$.

1.3. Organization. The structure of this paper is given as follows. In Section 2 we present the bilevel optimization problem of interest in a stochastic framework, and present a statistical consistency result of the adaptive parameter. We then extend this result to the linear inverse setting with Tikhonov regularization. This will lead onto Section 3 where we discuss the stochastic gradient descent method and its application in our bilevel optimization problem. We provide various assumptions required where we tend show in the linear setting that our parameter converges in $L_2$ to the minimizer. In Section 4 we test our theory on various numerical models which include both linear and nonlinear models such as Darcy flow and the eikonal equation. This will also include an image denoising example. Finally, we conclude our findings in Section 5. The appendix will contain the proofs for results in Section 2 and Section 3.

2. Regularization parameter offline recovery

In this section we discuss how to use offline bilevel optimization to recover regularization parameters. We also show the solution is statistically consistent under suitable conditions.

2.1. Offline bilevel optimization. Regularization parameter learning by bilevel optimization views the unknown parameter $U$ and the data $Y$ as a jointly distributed random variable with distribution $\mu_{(U,Y)}$, see e.g. [2] for more details. Recall the bilevel optimization problem is given by

$$\lambda_* = \arg\min_{\lambda \in \Lambda} F(\lambda), \quad F(\lambda) = \mathbb{E}_{\mu_{(U,Y)}}[L_U(u_\lambda(Y), U)], \quad \text{(upper level)}$$

$$u_\lambda(Y) := \arg\min_{u \in U} \Psi(\lambda, u, Y), \quad \Psi(\lambda, u, y) := L_Y(G(u), y) + S_\lambda(u), \quad \text{(lower level)}$$
where $\mathcal{L}_U$ denotes a discrepancy function in the parameter space $\mathcal{U} := \mathbb{R}^d$ and $\mathcal{L}_Y$ denotes a discrepancy function in the observation space $\mathcal{Y} := \mathbb{R}^K$. $S_\lambda(U)$ represents the regularization with parameter $\lambda \in \Lambda$. Here, $\Lambda$ represents the range of regularization parameters which often come from physical constraints. For simplicity, we assume all the functions here are continuous and integrable, and so are their first and second order derivatives with respect to $\lambda$.

In general, we do not know the exact distribution $\mu$ in the upper level of (1.3). We consider the scenario where we have access to training data $(u^{(i)}, y^{(i)})_{i=1}^n$, which we assume to be i.i.d. samples from $\mu(U,Y)$. With these data, we can approximate $F$ in (1.3) by its empirical average:

$$\hat{F}_n = \frac{1}{n} \sum_{j=1}^n \mathcal{L}_U(u_\lambda(y^{(j)}), u^{(j)}).$$

This leads to a data-driven estimator of the regularization parameter,

$$\hat{\lambda}_n = \arg\min_{\lambda \in \Lambda} \hat{F}_n,$$

$$u_\lambda(y^{(j)}) = \arg\min_{u \in \mathcal{U}} \mathcal{L}_Y(\hat{G}(u), y^{(j)}) + S_\lambda(u).$$

This method of estimation is often known as empirical risk minimization in machine learning [47]. We refer to this as “offline” since minimizing $\hat{F}_n$ involves all $n$ data points at each algorithmic iteration. With $\hat{\lambda}_n$ being formulated, it is of natural interest to investigate its convergence to the true parameter $\lambda_*$, when the sample size increases. Consistency analysis is of central interest in the study of statistics. In particular, if $\hat{\lambda}_n$ is the global minimum of $\hat{F}_n$, we have the following theorem.

**Theorem 2.1.** Suppose for any $\epsilon > 0$

$$\mathbb{P}(\sup\{\lambda \in \Lambda, |\hat{F}_n(\lambda) - F(\lambda)| > \epsilon\} \to 0,$$

as $n \to \infty$, $\hat{\lambda}_n$ is the global minimizer of $\hat{F}_n$, and $\lambda_*$ is the unique minimizer of $F$, then $\hat{\lambda}_n$ is a consistent estimator.

In more practical scenarios, the finding of $\hat{\lambda}_n$ relies on the choice of optimization algorithms. If we are using gradient based algorithms, such as gradient descent, $\hat{\lambda}_n$ can be the global minimum of $\hat{F}_n$ if $\hat{F}_n$ is convex. More generally, we can only assume $\hat{\lambda}_n$ to be a stationary point of $\hat{F}_n$, i.e. $\nabla \hat{F}_n(\hat{\lambda}_n) = 0$. In such situations, we provide the following alternative tool replacing Theorem 2.1:

**Proposition 2.2.** Suppose $F$ is $C^2$, $\lambda_*$ is a local minimum of $F$, and $\hat{\lambda}_n$ is a local minimum of $\hat{F}_n$. Let $\mathcal{D}$ be an open convex neighborhood of $\lambda_*$ in the parameter space and $c_0$ be a positive constant. Denote $\mathcal{A}_n$ as the event

$$\mathcal{A}_n = \{\hat{\lambda}_n \in \mathcal{D}, \nabla_\lambda^2 \hat{F}_n(\lambda) \succeq c_0 I \text{ for all } \lambda \in \mathcal{D}\}.$$

When $\mathcal{A}_n$ takes place, the following holds:

$$\|\hat{\lambda}_n - \lambda_*\| \leq \frac{\|\nabla_\lambda \hat{F}_n(\lambda_*) - \nabla_\lambda F(\lambda_*)\|}{c_0}.$$

In particular, we have

$$\mathbb{E}1_{\mathcal{A}_n} \|\hat{\lambda}_n - \lambda_*\| \leq \frac{\sqrt{\text{tr}(\text{Var}(\nabla_\lambda f(\lambda_*, Z)))}}{c_0 \sqrt{n}}.$$

Proposition 2.2 makes two claims. From the second claim, we can see $\lambda_n$ converges to $\lambda_*$ at rate of $\frac{1}{\sqrt{n}}$. And with the first claim, sometimes we can have more
accurate estimate on large or medium deviations. We will see how to do that in the linear inverse problem discussed below.

On the other hand, Proposition 2.2 requires the existence of region \( \mathcal{D} \) so that both \( \hat{\lambda}_n \) and \( \lambda^* \) are in it, moreover \( \hat{F}_n \) needs to be strongly convex inside \( \mathcal{D} \). The convexity part is necessary, since without it, there might be multiple local minimums, and we will have identifiability issues. In order to apply Theorem 2.2, one needs to find \( \mathcal{D} \) and bound the probability of outlier cases \( A_n^c \). This procedure can be nontrivial, and requires some advanced tools from probability. We demonstrate how to do so for the linear inverse problem.

2.2. Offline consistency analysis with linear observation models. In this section we demonstrate how to apply Theorem 2.2 for linear observation models with Tikhonov regularization. In particular, we assume \( u \in \mathbb{R}^d \) and the data \( y \) is observed through a matrix \( A \in \mathbb{R}^{K \times d} \).

\[
y = Au + \eta,
\]

with Gaussian prior information \( u \sim \mathcal{N}(0, \frac{1}{\lambda} C_0) \) and Gaussian noise \( \xi \sim \mathcal{N}(0, \Gamma) \). The common choice of discrepancy functions in the lower level are the corresponding negative log-likelihoods

\[
L_y(G(u), y) = \frac{1}{2} \| Au - y \|^2, \quad S_\lambda(u) = \frac{\lambda}{2} \| u \|_2^2.
\]

Since both of these functions are quadratic in \( u \), the lower level optimization problem has an explicit solution

\[
u_\lambda(y) = (A^\top \Gamma^{-1} A + \lambda C_0)^{-1} A^\top \Gamma^{-1} y.
\]

If we use the root-mean-square error in the upper level to learn \( \lambda \), the discrepancy function is given by

\[
f(\lambda, u, y) = \| u_\lambda(y) - u \|^2.
\]

and the empirical loss function is defined by

\[
\hat{F}_n(\lambda) = \frac{1}{n} \sum_{i=1}^{n} \| u_\lambda(y_i) - u_i \|^2.
\]

It is worth mentioning that \( F(\lambda) \) is not convex on the real line despite that \( G \) is linear. The detailed calculation can be found in Remark A.3. It is of this reason, it is necessary to introduce the local region \( \mathcal{D} \) that \( F \) is convex inside at Proposition 2.2.

Since the formulation of \( u_\lambda \) involves the inversion of matrix \( A^\top \Gamma^{-1} A + \lambda C_0 \), such an operation may be unstable for \( \lambda \) approaching \( \infty \). When \( \lambda \) approaches \( \infty \), the gradient of \( \hat{F}_n \) approaches zero, so \( \infty \) can be a stationary point that an optimization algorithm tries to converge to. To avoid these issues, we assume there are lower and upper bounds such that

\[
0 < \lambda_l < \frac{1}{2} \lambda_* < \frac{3}{2} \lambda_* < \lambda_u,
\]

where \( \lambda_l \) can be chosen as a very small number and \( \lambda_u \) can be very large. Their values often can be obtained from physical restrictions from the inverse problem. By assuming their existence, we can restrict \( \lambda_n \) to be in the interval \( \Lambda = (\lambda_l, \lambda_u) \).

Now we are ready to present our main result for the offline recovery of regularization parameter. In particular, we show \( \tilde{\lambda}_n \) converges to \( \lambda_* \) with high probability.

**Theorem 2.3.** Suppose \( \lambda_n^* \in (\lambda_l, \lambda_u) \) is a local minimum of \( \hat{F}_n \). Then there exist \( C_*, c_* > 0 \) such that for any \( 1 \geq \epsilon > 0 \) and \( n \),

\[
\mathbb{P}(|\tilde{\lambda}_n - \lambda_*| > \epsilon, \lambda_l < \tilde{\lambda}_n < \lambda_u) \leq C_* \exp(-c_* n \min(\epsilon, \epsilon^2)).
\]
The values of \( C_*, c_0 > 0 \) depend on \( \lambda_l, \lambda_u, \lambda_*, C_0 \) but not on \( n \).

Since we can obtain consistency assuming that \( \hat{\lambda}_n \) is a local minimum, we do not demonstrate how to implement Theorem 2.1 for the more restrictive scenario where \( \hat{\lambda}_n \) is a global minimum.

Remark 2.4. We note that in the Gaussian setting with Tikhonov regularization one can also estimate \( \lambda_\ast \) empirically by using the maximum likelihood estimator

\[
\hat{\lambda}_n = d \cdot \left( \frac{1}{n} \sum_{j=1}^{n} (u^{(j)})^\top C_0^{-1} u^{(j)} \right)^{-1}.
\]

However, only in the Gaussian setting with Tikhonov regularization the estimate will lead to the optimal solution of (1.3). When considering alternative regularization, or dropping the Gaussian assumption on \( u \), it is not clear whether this approach still leads to a good estimate of \( \lambda_\ast \).

3. Regularization parameter online recovery

In this section we discuss how to implement the stochastic gradient descent (SGD) method for online solutions of the bilevel optimization. We will formulate the SGD method for general nonlinear inverse problems and state certain assumptions on the forward model and the regularization function to ensure convergence of the proposed method.

3.1. Bilevel stochastic gradient descent method. In the offline solution of the bilevel optimization problem (2.2), one has to compute the empirical loss function \( \hat{F}_n \) or its gradient in (2.1). This involves solving the lower level problem for each training data point \( (u^{(j)}, y^{(j)}), j = 1, \ldots, n \). When \( n \) is very large, this can be very computationally demanding. One way to alleviate this is to use the stochastic gradient descent (SGD). This has been done in the context of traditional optimization [16], where various convergence results were shown. As a result this has been applied to problems in machine learning, most notably support vector machines [14, 15], but also in a more general context without the use of SGD [25, 31]. Here we propose a SGD method to solve the bilevel optimization problem (1.3) online.

To formulate the SGD method, we first note that the gradient descent method generates iterates \( \lambda_{k+1} \) based on the following update rules

\[
\lambda_{k+1} = \lambda_k - \beta_k \nabla_\lambda F(\lambda_k),
\]

where \( \beta_k \) is a sequence of stepsizes.

As mentioned above, the population gradient \( \nabla_\lambda F \) is often computationally inaccessible, and its empirical approximation \( \nabla_\lambda \hat{F}_n \) is often expensive to compute. One general solution to this issue is using a stochastic approximation of \( \nabla_\lambda F \). Here we choose \( \nabla_\lambda f(\lambda_k, Z^{(k)}) \), since it is an unbiased estimator of \( \nabla_\lambda F \):

\[
\nabla_\lambda F(\lambda_k) = \mathbb{E}_Z \nabla_\lambda f(\lambda_k, Z).
\]

The identity above holds by Fubini’s theorem, since we assume \( f \) and its second order derivatives are all continuous and differentiable. Comparing with \( \nabla_\lambda \hat{F}_n, \nabla_\lambda f \) involves only one data point \( Z^{(k)} \), so it has a significantly smaller computation cost. We refer to this method as “online”, since it does not require all \( n \) data points available at each algorithmic iteration.

We formulate the stochastic gradient descent method to solve (1.3) as Algorithm 1.
Lemma 3.2. Suppose the lower level loss function \( \psi(\lambda, u, y) \) is \( C^2 \) and strictly convex for \((u_{\lambda_0}, \lambda_0)\), then the function \( \lambda \mapsto u_{\lambda}(y) \) is continuously differentiable w.r.t. \( \lambda \) near \( \lambda_0 \) and the derivative is given by
\[
\nabla_{\lambda} u_{\lambda}(y) = - (\nabla^2_u [\psi(\lambda, u_{\lambda}(y), y)])^{-1} \nabla^2_{\lambda u} [\psi(\lambda, u_{\lambda}(y), y)].
\]

3.2. **Approximate stochastic gradient method.** In order to implement Algorithm 1, it is necessary to evaluate the gradient \( \nabla_{\lambda} f \). While Lemma 3.2 provides a formula to compute the gradient, its evaluation can be expensive for complicated PDE forward models. In these scenarios, it is more reasonable to implement approximate SGD.

One general way to find approximate gradient is applying central finite difference schemes. This involves perturbing certain coordinates in opposite direction, and use the value difference to approximate the gradient:
\[
(\widetilde{\nabla}_{\lambda} f(\lambda_k, z))_i \approx \frac{f(\lambda_k + h_k e_i, z) - f(\lambda_k - h_k e_i, z)}{2h_k},
\]
where \( e_i \) is the \( i \)-th Euclidean basis vector and \( h_k \) is a step size. \( h_k \) can either be fixed as a small constant, or it can be decaying as \( k \) increases, so that higher accuracy gradients are used when the iterates are converging.
In many cases, the higher level optimization uses a $L_2$ loss function
\[ \mathcal{L}_{uf}(y, u) = \|y - u\|^2. \]
The exact SGD update step (3.1) can be written as
\[ \lambda_{k+1} = \lambda_k - \beta_k \nabla \|u_{\lambda_k}(y^{(k)}) - u^{(k)}\|^2 \]
\[ = \lambda_k - \beta_k \left( \nabla_{\lambda} u_{\lambda_k}(y^{(k)}) \right) ^\top (u_{\lambda_k}(y^{(k)}) - u^{(k)}). \]
In this case, it makes more sense to apply central difference scheme only on the $\nabla u_{\lambda}$ part:
\[
(\nabla_{\lambda} u_{\lambda}(y^{(k)}))_i = \frac{\partial u_{\lambda}(y^{(k)})}{\partial \lambda_i} \approx \frac{u_{\lambda+h_k \varepsilon_i}(y^{(k)}) - u_{\lambda-h_k \varepsilon_i}(y^{(k)})}{2h_k} =: (\tilde{\nabla}_{\lambda} u_{\lambda}(y^{(k)}))_i,
\]
where $(\varepsilon_i)_{i=1,...,d}$ denote the $i$-th unit vectors in $\mathbb{R}^d$. Using this approximation, we formulate the approximate SGD method in the following algorithm, where we replace the exact gradient $\nabla_{\lambda} u_{\lambda}(y^{(k)})$ by the numerical approximation $\tilde{\nabla}_{\lambda} u_{\lambda}(y^{(k)})$ defined in (3.5).

Here we have defined the numerical approximation of $\nabla_{\lambda} f$ by
\[
\tilde{\nabla}_{\lambda} f(\lambda, (y, u)) := \left( \tilde{\nabla}_{\lambda} u_{\lambda}(y) \right) ^\top (u_{\lambda}(y) - u).
\]
In most finite difference approximation schemes, the approximation error involved is often controlled by $h_k$. In particular, we assume the centred forward difference scheme used in either (3.4) or (3.6) yields an error of order
\[ \|\mathbb{E} \tilde{\nabla}_{\lambda} f(\lambda, Y, U) \| =: \alpha_k = O(h_k^2). \]
Replacing the stochastic gradient in Algorithm 1 with its approximation, we obtain the algorithm below:

**Algorithm 2** Approximate Bilevel Stochastic Gradient Descent

1. Input: $\lambda_0$, $m$, $\beta = (\beta_k)_{k=1}^\infty$, $\beta_k > 0$, i.i.d. sample $(Z^{(k)})_{k \in \{1,...,n\}} \sim \mu(U,Y)$.
2. for $k = 0, \ldots, n - 1$ do
3.     $\lambda_{k+1} = \lambda_k - \beta_k \tilde{\nabla}_{\lambda} f(\lambda_k, Z^{(k)}),$
4. end for
5. Output: the average $\bar{\lambda}_n = \frac{1}{m} \sum_{k=n-m+1}^n \lambda_k$

### 3.3. Consistency analysis for online estimators.

Next we formulate sufficient conditions that can ensure that $\lambda_k$ converges in $L^2$ to the optimal solution $\lambda_*$ of (1.3).

**Proposition 3.3.** Suppose that there is a convex region $\mathcal{D} \subset \Lambda$ and a constant $c > 0$ such that
\[
\inf_{\lambda \in \mathcal{D}} (\lambda - \lambda_*)^\top \nabla \lambda F(\lambda) > c\|\lambda - \lambda_*\|^2.
\]
and there are constants $a$, $b > 0$ such that for all $\lambda \in \mathcal{D}$ it holds true that
\[
\mathbb{E} [\|\tilde{\nabla}_{\lambda} f(\lambda, Z)\|^2] < a + b\|\lambda - \lambda_*\|^2.
\]
Also the bias in the approximated SGD is bounded by
\[
\|\mathbb{E} \tilde{\nabla}_{\lambda} f(\lambda_k, Z_k) - \nabla \lambda F(\lambda_k)\|^2 \leq \alpha_k.
\]
Let $A_n$ be the event that $\lambda_k \in \mathcal{D}$. Suppose $\beta_0 \leq \frac{c}{b}$. Then if the approximation error is bounded by a small constant $\alpha_k \leq \alpha_0$, there is a constant $C_n$ such that

$$
\mathbb{E}1_{A_n} \|\lambda_n - \lambda_*\|^2 \leq \left( \mathbb{E}Q_0 + 2\alpha \sum_{j=1}^{\infty} \beta_j^2 \right) C_n + \frac{\alpha_0}{c^2}.
$$

Here

$$
C_n = \min_{k \leq n} \max \left\{ \prod_{j=k+1}^{n} (1 - c\beta_j), \alpha \beta_k/c \right\}
$$
is a sequence converging to zero.

If the approximation error is decaying so that $\alpha_k \leq D\beta_k$, then we have the estimation error

$$
\mathbb{E}1_{A_n} \|\lambda_n - \lambda_*\|^2 \leq \left( \mathbb{E}Q_0 + 2(a + D/c) \sum_{j=1}^{\infty} \beta_j^2 \right) C_n.
$$

**Remark 3.4.** We note that the above result also leads to similar convergence of the average estimator $\bar{\lambda}_n$ since by Jensen’s inequality

$$
\|\bar{\lambda}_n - \lambda_*\|^2 \leq \frac{1}{m} \sum_{k=n-m+1}^{n} \|\lambda_k - \lambda_*\|^2.
$$

Further, for standard SGD methods the averaging step has been shown to lead to the highest possible convergence rate under suitable assumptions. Interested readers can refer to [40] for more details.

### 3.4. Consistency analysis with linear inverse problem.

We consider again the linear inverse problem from Section 2.2

$$
y = Au + \xi,
$$

with Gaussian prior information $u \sim \mathcal{N}(0, \frac{1}{\lambda} C_0)$ and Gaussian noise $\xi \sim \mathcal{N}(0, \Gamma)$, and the corresponding bilevel optimization with least squares data misfit and Tikhonov regularization, i.e.

$$
\mathcal{L}_y(Au, y) = \frac{1}{2} \|Au - y\|_F^2, \quad S_\lambda(u) = \frac{\lambda}{2} \|u\|_{C_0}^2.
$$

**Theorem 3.5.** Let $\beta = (\beta_k)_{k \in \mathbb{N}}$ be a sequence of step sizes with $\beta_k > 0$, $\sum_{k=1}^{\infty} \beta_k = \infty$, and $\sum_{k=1}^{\infty} \beta_k^2 < \infty$. Then for some constant $B$ and a sequence $C_n$ converging to zero, the following hold

1. the iterates generated from the exact SGD, Algorithm 1, converge to $\lambda_*$ in the sense

$$
\mathbb{E} \|\lambda_n - \lambda_*\|^2 \leq BC_n.
$$

2. the iterates generated from the approximate SGD, Algorithm 2 with formula (3.6) and $h_k = h$, converge to $\lambda_*$ up to an error of order $\mathcal{O}(h^4)$, i.e.

$$
\mathbb{E} \|\lambda_n - \lambda_*\|^2 \leq B(C_n + h^4).
$$

If we use decaying finite difference stepsize $h_k \leq h \beta_k^{1/4}$, then the error can be further bounded by

$$
\mathbb{E} \|\lambda_n - \lambda_*\|^2 \leq BC_n.
$$
Remark 3.6. While in the offline setting the proof of the consistency result for the linear Gaussian setting was heavily relying on the Gaussian assumption on \( u \) and \( \xi \), in the online setting we are able to extend the result to non Gaussian distributions of \( u \) and \( \xi \). For our proof of Theorem 3.5 in Appendix B.3 we only need to assume that \( \mathbb{E}[|u|^4] < \infty \) and \( \mathbb{E}[|A^\top \Gamma^{-1} \xi|^4] < \infty \). Hence, it can also be applied to general linear inverse problems without Gaussian assumption on the unknown parameter or Gaussian assumption on the noise.

4. Numerical results

In this section our focus will be directed on testing the results of the previous sections. We will present various inverse problems to our theory, which will be based on partial differential equations, both linear and nonlinear which includes a linear 2D Laplace equation, a 2D Darcy flow from geophysical sciences and a 2D eikonal equation which arises in wave propagation. As a final numerical experiment, related to the examples discussed in Section 1, we test our theory on an image denoising problem.

For the linear example, we have access to the exact derivative of the Tikhonov solution for the bilevel optimization. In particular, we can implement both offline and online bilevel optimization methodologies. In contrast, finding the exact derivatives for nonlinear inverse problems is difficult both in derivation and computation, so we will only use online methods with approximated gradient. For online methods, we implement the following variants:

- **bSGD**: Application of the bilevel SGD, Algorithm 1 with exact derivative (3.3).
- **bSGD_a**: Application of the bilevel SGD, Algorithm 2 with derivative approximation (3.6) for fixed \( h_k = h_0 \) in (3.5).

For our first model we have tested both bSGD and bSGD_a, while for the nonlinear models we have used bSGD_a. It is worth mentioning that we have also tested, as a side experiment, using the adaptive derivative \( h_k = h_0 / k^{3/4} \). For these experiments it was shown that the adaptive derivative scheme does not show any major difference to the case of fixed \( h_k = h_0 \). In fact, Theorem 3.5 has already implied this, since the difference between the two scheme is of order \( h_0^{-4} \), which is often smaller than the error from the numerical forward map solver or the use of \( \lambda_0 \). For this reason, we do not demonstrate this scheme in our numerics.

4.1. Linear example: 2D Laplace equation. We consider the following forward model

\[
\left\{ \begin{array}{ll}
-\Delta p(x) &= u(x), & x \in X, \\
p(x) &= 0, & x \in \partial X,
\end{array} \right.
\]

with Lipschitz domain \( X = [0, 1]^2 \) and consider the corresponding inverse problem of recovering the unknown \( u^\dagger \) from observation of (4.1), described through

\[
y = \mathcal{O}(p) + \eta,
\]

where \( \eta \sim \mathcal{N}(0, \Gamma) \) is measurements noise and \( p \) is the solution of (4.1). We solve the PDE in weak form, where \( A^{-1} : \mathcal{U} \to \mathcal{V} \), with \( \mathcal{U} = L^\infty(X) \) and \( \mathcal{V} = H^2_0(X) \cap H^2(X) \), denotes the solution operator for (4.1) and \( \mathcal{O} : \mathcal{V} \to \mathbb{R}^K \) denotes the observation map taking measurements at \( K \) randomly chosen points in \( X \), i.e. \( \mathcal{O}(p) = (p(x_1), \ldots, p(x_K))^\top \), for \( p \in \mathcal{V}, x_1, \ldots, x_K \in X \). For our numerical setting \( K = 250 \) points have been observed, which is illustrated in Figure 1. We can express this problem as a linear inverse problem in the reduced form (2.3) by

\[
y^\dagger = Au^\dagger + \eta \in \mathbb{R}^K,
\]
where \( A = O \circ A^{-1} \) is the forward operator which takes measurements of (4.1). The forward model (4.1) is solved numerically on a uniform mesh with 1024 grid points in \( \mathcal{X} \) by a finite element method with continuous, piecewise linear finite element basis functions.

We assume that our unknown parameter \( u \) follows a Gaussian distribution \( \mathcal{N}(0, C_0) \) with covariance

\[
C_0 = \beta \cdot (\tau^2 I - \triangle)^{-\alpha},
\]

with Laplacian operator \( \triangle \) equipped with Dirichlet boundary conditions, known \( \beta, \tau > 0, \alpha > 1 \) and unknown \( \lambda^* > 0 \). To sample from the Gaussian distribution, we consider the truncated Karhunen-Loève (KL) expansion \([36]\), which is a series representation for \( u \sim \mathcal{N}(0, C_0) \), i.e.

\[
u(x) = \sum_{i=1}^{\infty} \frac{\xi_i}{\lambda_i} \sigma_i \varphi_i(x),
\]

where \( \sigma_i, \varphi_i \) are the eigenvalues and eigenfunction of the covariance operator \( C_0 \) and \( \xi = (\xi_i)_{i \in \mathbb{N}} \) is an i.i.d. sequence with \( \xi_1 \sim \mathcal{N}(0, 1) \) i.i.d. Here, we have sampled from the KL expansion for the discretized \( C_0 \) on the uniform mesh. Furthermore, we assume to have access to training data \( (u^{(j)}, y^{(j)})_{j=1,\ldots,n} \), \( n \in \mathbb{N} \), which we will use to learn the unknown scaling parameter \( \lambda^* \) before solving the inverse problem. For the numerical experiment we set \( \beta = 100, \tau = 0.1, \alpha = 2 \) and \( \lambda = 0.1 \). After learning the regularization parameter, we will compare the estimated parameter through the different results of the Tikhonov minimum

\[
u_{\lambda_i}(y^{(j)}) = (A^\top \Gamma_i^{-1} A + \lambda_i \cdot C_0)^{-1} A^\top y^{(j)},
\]

for \( \lambda = \hat{\lambda} \) learned from the training data, \( \lambda_2 = \lambda_3 \), and fixed \( \lambda_3 = 1 \). We have used the MATLAB function \texttt{fmincon} to recover the the regularization parameter offline by solving the empirical optimization problem

\[
\hat{\lambda}_n \in \arg\min_{\lambda > 0} \frac{1}{n} \sum_{j=1}^{n} |u_{\lambda}(y^{(j)}) - u^{(j)}|^2.
\]

We use \( M = 1000 \) samples of training data to construct Monte–Carlo estimates of \( \mathbb{E}[|\lambda_n - \lambda^*|^2] \). While the computation of the empirical loss function can be computational demanding, we also apply the proposed online recovery in form of the SGD method to learn the regularization parameter \( \lambda \) by running Algorithm 1 with chosen step size \( \beta_k = 200/k \), range of regularization parameter \( \Lambda = [0.0001, 10] \) and initial value \( \lambda_0 = 1 \). The resulting iterate \( \lambda_k \) can be seen in Figure 2 on the right side.

From the numerical experiments for the linear example we observe that the numerics match our derived theory. In the offline recovery setting, this is first evident in Figure 2 on the left side. We compare the MSE with the theoretical rate, which seems to decay at the same rate. The online recovery is highlighted by the right plot in Figure 2 which demonstrates the convergence towards \( \lambda^* \) as the iterations progress. Further, we show the result of the approximate bSGD method Algorithm 2 for fixed chosen \( h_k = 0.01 \) in (3.5). As the derivative approximation (3.5) is closely exact, we see very similar good performance of the approximate bSGD method.

Finally, Figure 3 shows the recovery of the underlying unknown through different choices of \( \lambda \). It verifies that the adaptive learning of \( \lambda \) outperforms that of fixed regularization parameter \( \lambda = 1 \).
4.2. Nonlinear example: 2D Darcy flow. We now consider the following elliptic PDE which arises in the study of subsurface flow known as Darcy's flow. The forward model is concerned using the log-permeability $\log u \in L^\infty(X) =: \mathcal{U}$ to solve for the pressure $p \in H^1_0(X) \cap H^2(X) =: \mathcal{V}$ from

\begin{equation}
\begin{cases}
-\nabla \cdot (\exp(u)\nabla p) = f, & x \in X \\
p = 0, & x \in \partial X
\end{cases}
\end{equation}

with domain $X = [0,1]^2$ and known scalar field $f \in \mathbb{R}$. We again consider the corresponding inverse problem of recovering the unknown $u^\dagger$ from observation of (4.4), described through

\[ y = \mathcal{O}(p) + \eta, \]

where $\mathcal{O} : \mathcal{V} \to \mathbb{R}^K$ denotes the linear observation map, which takes again measurements at $K$ randomly chosen points in $X$, i.e. $\mathcal{O}(p) = (p(x_1), \ldots, p(x_K))^\top$, for $p \in \mathcal{V}, x_1, \ldots, x_K \in X$. For our numerical setting we choose $K = 125$ observational points, which can again be seen in Figure 4. The measurements noise is denoted by $\eta \in \mathcal{N}(0, \Gamma)$, for $\Gamma \in \mathbb{R}^{K \times K}$ symmetric and positive definite.

We formulate the inverse problem through

\[ y^\dagger = \mathcal{G}(u^\dagger) + \eta, \]
Figure 3. Comparison of different Tikhonov solutions for choices of regularization parameter $\lambda_i$. The learned Tikhonov regularized solution corresponds to the resulting one of the SGD method Algorithm 1 for the Laplace equation.

with $\mathcal{G} = \mathcal{O} \circ G$, where $G : \mathcal{U} \rightarrow \mathcal{V}$ denotes the solution operator of (4.4), solving the PDE (4.4) in weak form. The forward problem (4.4) has been solved by a second-order centered finite difference method on a uniform mesh with 256 grid points.

We assume that $u^\dagger$ follows the Gaussian distribution $\mathcal{N}(0,\frac{1}{\lambda^*}C_0)$ with a covariance operator (4.2) prescribed with Neumann boundary condition. Similar as before, $\beta, \tau > 0$ and $\alpha > 1$ are known, while $\lambda^* > 0$ is unknown. This time, in order to infer the unknown parameter, we use the KL expansion and do estimation of the coefficients $\xi$. See also [10, 27] for more details. Therefore we truncate (4.3) up to $d$ and consider the nonlinear map $\mathcal{G} : \mathbb{R}^d \rightarrow \mathbb{R}^K$, with $\mathcal{G}(\xi) = G(u^\xi(\cdot))$ and

$$u^\xi(\cdot) = \sum_{i=1}^{d} \xi_i \sqrt{\frac{1}{\lambda^*_i}} \sigma_i \varphi_i(\cdot).$$

This implies our unknown parameter is given by $\xi \in \mathbb{R}^d$ and we set a Gaussian prior on $\xi$ with $\mathcal{N}(0,\frac{1}{\lambda^*}I)$, where $\lambda^* > 0$ is unknown.

We again assume to have access to training data $(\xi(j),y(j))_{j=1,\ldots,n}$, $n \in \mathbb{N}$, where $\xi(j) \sim \Xi \sim \mathcal{N}(0,\frac{1}{\lambda^*}I)$ and we aim to solve the original bilevel optimization problem

$$\hat{\lambda} \in \arg\min_{\lambda > 0} \mathbb{E}[\|u_\lambda(Y) - \Xi\|^2], \quad u_\lambda(Y) = \arg\min_{\xi \in \mathbb{R}^d} \frac{1}{2} \|\mathcal{G}(\xi) - Y\|^2 + \frac{\lambda}{2} \|\xi\|^2.$$

The corresponding empirical optimization problem is given by (4.5)

$$\hat{\lambda}^n \in \arg\min_{\lambda > 0} \frac{1}{n} \sum_{j=1}^{n} \|u_\lambda(y(j)) - \xi(j)\|^2, \quad u_\lambda(y(j)) = \arg\min_{\xi \in \mathbb{R}^d} \frac{1}{2} \|\mathcal{G}(\xi) - y(j)\|^2 + \frac{\lambda}{2} \|\xi\|^2,$$
for a given size of the training data \( n \). In comparison to the linear setting, we are not able to compute the Tikhonov minimum analytically for each observation \( y^{(j)} \), as we require more computational power to solve (4.5). We will solve (4.5) online by application of Algorithm 2, where we will approximate the derivative of the forward model by centered different method (3.5). We keep the accuracy of the numerical approximation fixed to \( h_k = 0.01 \).

For our numerical results we choose \( d = 25 \) coefficients in the KL expansion and the noise covariance \( \Gamma = \gamma^2 I \) with \( \gamma = 0.001 \). For the prior model set \( \beta = 10 \), \( \alpha = 2 \), \( \tau = 3 \) and the true scaling parameter \( \lambda^* = 0.1 \).

For the SGD method we have chosen a step size \( \beta_k = 0.001 k^{-1} \). The learned parameter moves fast into direction of the true \( \lambda^* \), and oscillates around this value, where the variance reduces with the iterations, as seen in Figure 6.

Finally, Figure 5 highlights again the importance and improvements of choosing the right regularization parameters.

4.3. Nonlinear example: Eikonal equation. We also seek to test our theory on the eikonal equation, which is concerned with wave propagation. Given a slowness or inverse velocity function \( s(x) \in C^0(\bar{X}) =: \mathcal{U} \), characterizing the medium, and a source location \( x_0 \in X \), the forward eikonal equation is to solve for travel time \( T(x) \in C^0(\bar{X}) =: \mathcal{V} \) satisfying

\[
\begin{align*}
|\nabla T(x)| &= s(x), \quad x \in X \setminus \{x_0\}, \\
T(x_0) &= 0, \\
\nabla T(x) \cdot \nu(x) &\geq 0, \quad x \in \partial X.
\end{align*}
\]

The forward solution \( T(x) \) represents the shortest travel time from \( x_0 \) to a point in the domain \( X \). The Soner boundary condition imposes that the wave propagates along the unit outward normal \( \nu(x) \) on the boundary of the domain. The model equation (4.6) is of the form (1.4) with an additional constrain arising from the Soner boundary condition.

The inverse problem for (4.6) is to determine the speed function \( s = \exp(u) \) from measurements of the shortest travel time \( T(x) \). The data is assumed to take the form

\[
y = \mathcal{O}(T) + \eta,
\]

where \( \mathcal{O} : \mathcal{V} \to \mathbb{R}^K \) denotes the linear observation map, which takes again measurements at \( K = 125 \) randomly chosen grid points in \( X \), i.e. \( \mathcal{O}(p) = (T(x_1), \ldots, T(x_K))^\top \).
Figure 5. Comparison of different Tikhonov solutions for choices of the regularization parameter $\lambda$. The learned Tikhonov regularized solution corresponds to the resulting one of the SGD method Algorithm 2 for Darcy flow.

Figure 6. Learned regularization parameter $\lambda_k$, for Darcy flow, resulting from the approximate bilevel SGD method Algorithm 2 with fixed derivative accuracy $h = h_0$ and the corresponding mean over the last 50 iterations $\bar{\lambda}_n$. We obtain an error $|\lambda^*_n - \bar{\lambda}_n|^2 = 3.3640e^{-05}$.

for $T \in Z, x_1, \ldots, x_K \in X$. The observed points can be seen in Figure 7. The measurements noise is again denoted by $\eta \in \mathcal{N}(0, \Gamma)$, for $\Gamma \in \mathbb{R}^{K \times K}$ symmetric and positive definite. Again we formulate the inverse problem through

$$y^\dagger = G(u^\dagger) + \eta,$$

with $G = \mathcal{O} \circ G$, where $G : \mathcal{U} \to \mathcal{V}$ denotes the solution operator of (4.4). As before we will assume our unknown $u^\dagger$ is distributed according to a mean-zero Gaussian with covariance structure (4.2). For this numerical example we set $\beta = 1, \tau = 0.1, \alpha = 2$ and $\lambda^*_n = 0.1$. We truncate the KL expansion such that the unknown parameters $\xi \in \mathbb{R}^d$ with $d = 25$. For the eikonal equation we take a similar approach.
to Section 4.2, that is we use the SGD described through Algorithm 2. For the SGD method we have chosen an adaptive step size

$$\beta_k = \min \left( 0.002, \frac{\lambda_0}{|\nabla f(\lambda_k, Z^{(k)})|} \right)^{k-1}. $$

Here, the chosen step size \( \beta_k \) provides a bound on the maximal moved step in each SGD step, i.e.

$$|\beta_k \cdot \nabla f(\lambda_k, Z^{(k)})| \leq \lambda_0/k.$$  

This helps to avoid instability arising through the high variance of the stochastic gradient, but the step size will be mainly of order 0.002/k. However, from theoretical side it is not clear whether assumption of (3.2) is still satisfied. Therefore, we will also show the resulting \( \sum_{k=1}^{n} \beta_k \) and the realisation of the stochastic gradient \( \nabla f(\lambda_k, Z^{(k)}) \) in Figure 10.

Our setting for the parameter choices of our prior and for the bilevel-optimization problem remain the same. To discretize (4.6) on a uniform mesh with 256 grid points we use a fast marching method, described by the work of Sethian [23, 44].

As we observe the numerical experiments, Figure 8 highlights that using the learned \( \lambda_n \) provides recoveries almost identical to that of using the true \( \lambda_* \). For both cases we see an improvement over the case \( \lambda = 1 \) which is what we expected and have seen throughout our experiments. This is verified through Figure 9 where we see oscillations of the learned \( \lambda_k \) around the true \( \lambda_* \), until approximately 100 iterations where it starts to become stable. Finally from Figure 10 we see that the summation of our choice \( \beta_k \) diverges, but not as quickly as the summation of the deterministic step size 0.002/k does, which is the implication of the introduced adaptive upper bound based on the size of the stochastic gradient \( \nabla f(\lambda_k, Z^{(k)}) \).

Figure 10 also shows the histogram of the stochastic gradient and its rare realized large values.

4.4. Signal denoising example. We now consider implementing our methods on image denoising, which is discussed in Section 1 and subsection 1.1.2. We are interested in denoising a 1D compound Poisson process of the form

$$u_t = \sum_{i=1}^{N_t} X_i,$$

Figure 7. Reference PDE solution for the eikonal equation of the underlying unknown parameter \( u^d \), and the corresponding randomized observation points \( x_1, \ldots, x_K \in X \).
Figure 8. Comparison of different Tikhonov solutions for choices of the regularization parameter $\lambda$. The learned Tikhonov regularized solution corresponds to the resulting one of the SGD method Algorithm 2 for the eikonal equation.

Figure 9. Learned regularization parameter $\lambda_k$ for the eikonal equation, resulting from the approximate bilevel SGD method Algorithm 2 with fixed derivative accuracy $h = h_0$ and the corresponding mean over the last 50 iterations $\bar{\lambda}_n$. We obtain an error $|\lambda_* - \bar{\lambda}_n|^2 = 1.9360e-05$.

where $(N_t)_{t \in [0, T]}$ is a Poisson process, with rate $r > 0$ and $(X_i)_{i=1}^{N_t}$ are i.i.d. random variables representing the jump size. Here, we have chosen $X_1 \sim N(0, 1)$. We consider the task of recovering a perturbed signal of the form (4.7) through Tikhonov regularization with different choices of regularization parameter $\lambda$. In particular, the observed signal $u = (u_1, \ldots, u_d)^\top \in \mathbb{R}^d$ is perturbed by white noise

(4.8) $y_{t_i} = u_{t_i} + \eta_{t_i},$

where $t_i \in \{1/d \cdot T, 2/d \cdot T, \ldots, T\}$ and $\eta_{t_i} \sim N(0, \sigma^2)$ are i.i.d. random variables, and the Tikhonov estimate corresponding to the lower level problem of (1.5) for
Figure 10. Summation of the realized adaptive step size (left) and the realized stochastic gradient $\nabla f(\lambda_{k}, Z^{(k)})$ (right) resulting from the online recovery, Algorithm 1 for the eikonal equation.

| $\lambda$ | $1e-02$ | $1e-05$ | $\lambda_{in}$ | $\lambda_{o}$ |
|-----------|---------|---------|----------------|-------------|
| error     | 0.0378  | 0.0134  | 0.0077         | 0.0073      |

Table 1. MSE over time of the reconstruction for different choices of the regularization parameter for signal denoising example.

Given regularization parameter $\lambda > 0$ is defined by

$$u_{\lambda}(y) = (\Gamma^{-1} + \lambda L^{-1})^{-1}\Gamma^{-1}y,$$

with given regularization matrix $L \in \mathbb{R}^{d \times d}$ and $y = (y_{1}, \ldots, y_{d})^T \in \mathbb{R}^{d}$. We assume to have access to training data $(u^{(j)}), y^{(j)})_{j=1}^{n}$ of (4.8) and choose the regularization parameter $\hat{\lambda}$ according to Algorithm 1. Further, we compare the resulting estimate of the signal

$$y_{obs} = u^{\dagger} + \eta,$$

to fixed choices of $\lambda \in \{0.01, 0.00001\}$ and to the best possible choice $\lambda_{*} = \arg\min_{\lambda} \|u_{\lambda}(y_{obs}) - u^{\dagger}\|^2$.

For the experiment we set the rate of jumps $r = 10$ and consider the signal observed up to time $T = 1$ at $d = 1000$ observation points. For Algorithm 1, we use a training data set of size $n = 500$, we set an initial value $\lambda_{0} = 0.001$ and step size $\beta_{k} = 0.001k^{-1}$. The Tikhonov solution (4.9) has been computed with a second-order regularization matrix $L = \Delta^{-1}$. As we can see from our results the value of $\lambda = 0.001$ oversmoothes the estimate in comparison with $\lambda = 0.00001$. This is shown in Figure 11. However comparing fixed $\lambda$ with the learned $\lambda$ in Figure 12 we see an improvement, closer to the best possible $\lambda$, which is verified further through Table 1, where we can see the MSE over the time intervall. Both Figure 11 and Figure 12 show on the right hand side the pointwise squared error over time.

5. Conclusion

In this work we have provided new insights into the theory of bilevel learning for inverse problems. In particular our focus was on deriving statistical consistency results with respect to the data limit of the regularization parameter $\lambda$. This was considered for both the offline and online representations of the bilevel problem. For the online version we used and motivated stochastic gradient descent as the choice of optimizer, as it is well known to reduce the computational time required compared to other methodologies. To test our theory we ran numerical experiments on various PDEs which not only verified the theory, but clarified that adapting the
Figure 11. Comparison of different Tikhonov solutions for fixed choices of the regularization parameter $\lambda$ for the signal denoising example.

Figure 12. Comparison of the learned to best possible Tikhonov solutions for choices of the regularization parameter $\lambda$. The learned Tikhonov regularized solution corresponds to the resulting one of the SGD method Algorithm 1 for the signal denoising example.

The regularization parameter $\lambda$ outperforms that of a fixed value. Our results in this article provide numerous directions for future, both practically and analytically.

- One direction is to consider a fully Bayesian approach, or understanding, to bilevel learning. In the context of statistical inverse problems, this could be related to treating $\lambda$ as a hyperparameter of the underlying unknown.
This is referred to as hierarchical learning \cite{39} which aims to improve the overall accuracy of the reconstruction \cite{1, 22}.

- Another potential direction is to understand statistical consistency from other choices of regularization. Answering this for other penalty terms, such as \(L_1\), total variation and adversarial \cite{38} (based on neural networks), is of importance and interest in numerous applications \cite{2}. A potential first step in this direction would be to consider the well-known elastic-net regularization \cite{24}, which combines both \(L_1\) and Tikhonov regularization. Of course to consider this one would need to modify the assumptions on convexity.

- Finally one could propose using alternative optimizers, which provide a lower computational cost. A natural choice would be derivative-free optimization. One potential optimizer could be ensemble Kalman inversion, a recent derivative-free methodology, which is of particular interest to the authors. In particular as EKI has been used in hierarchical settings \cite{10, 11}, the reduction in cost could be combined with the hierarchical motivation discussed above.

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Appendix A. Proofs of offline consistency analysis

A.1. General framework. We start with the proof for the general framework:

Proof of Proposition 2.2. To simplify the mathematical notation, we use \(z\) to denote the data couple \((u, y)\), and use \(f\) to denote the data loss function

\[ f(\lambda, z) = \mathcal{L}_t(u\lambda(y), u). \]

When \(\hat{\lambda}_n \in \mathcal{D}\), we apply the fundamental theorem of calculus on \(\nabla_\lambda \hat{F}_n\), and find

\[ \nabla_\lambda \hat{F}_n(\lambda_*) = \nabla_\lambda \hat{F}_n(\hat{\lambda}) + \int_0^1 \nabla^2_\lambda \hat{F}_n(s\lambda_* + (1-s)\hat{\lambda})(\lambda_* - \hat{\lambda}_n)ds = A_F(\hat{\lambda}_n - \lambda_*), \]

where

\[ A_F := \int_0^1 \nabla^2_\lambda \hat{F}_n((1-s)\hat{\lambda}_n + s\lambda_*)ds \geq c_0 I. \]

Note that

\[ \theta = \nabla_\lambda F(\lambda_*) = \nabla_\lambda F(\lambda_*) - \nabla_\lambda \hat{F}_n(\lambda_*) + \nabla_\lambda \hat{F}_n(\lambda_*) \]

\[ = A_F(\hat{\lambda}_n - \lambda_*) + \nabla_\lambda F(\lambda_*) - \nabla_\lambda \hat{F}_n(\lambda_*). \]

We can reorganize this as

\[ -\left( \nabla_\lambda \hat{F}_n(\lambda_*) - \nabla_\lambda F(\lambda_*) \right) = A_F(\hat{\lambda}_n - \lambda_*), \]

As a consequence, we now have a formula for the point estimation error \(
\lambda_* - \hat{\lambda}_n. \)

\[ \|
\lambda_* - \hat{\lambda}\| = \left\| A_F^{-1} \left( \nabla_\lambda \hat{F}_n(\lambda_*) - \nabla_\lambda F(\lambda_*) \right) \right\| \leq c_0^{-1} \left\| \nabla_\lambda \hat{F}_n(\lambda_*) - \nabla_\lambda F(\lambda_*) \right\|. \]
Note that by using $\nabla_\lambda \mathbb{E} f(\lambda, Z) = \mathbb{E} \nabla_\lambda f(\lambda, Z)$, see [43, Theorem 12.5],
\[ \nabla_\lambda \widehat{F}_n(\lambda_*) - \nabla_\lambda F(\lambda_*) = \frac{1}{n} \sum_{i=1}^{n} \nabla_\lambda f(\lambda_*, z_i) - \mathbb{E} \nabla_\lambda f(\lambda_*, Z). \]
So
\[ \mathbb{E} \| \nabla_\lambda \widehat{F}_n(\lambda_*) - \nabla_\lambda F(\lambda_*) \|^2 = \frac{1}{n} \text{tr}(\text{Var}(\nabla_\lambda f(\lambda_*, Z))). \]
And our second claim follows by Cauchy-Schwarz.
\[ \mathbb{E} \left\| \nabla_\lambda \widehat{F}_n(\lambda_*) - \nabla_\lambda F(\lambda_*) \right\|^2 \leq \sqrt{\mathbb{E} \| \nabla_\lambda \widehat{F}_n(\lambda_*) - \nabla_\lambda F(\lambda_*) \|}^2. \]

\[ \square \]

Next, we apply Proposition 2.2 to linearize the inverse problem. To simplify the discussion, we do a whitening transformation, $u_i = C_0^{-1/2} u_i$, such that we can assume w.l.o.g. $C_0 = \lambda^{-1} I$. Denote $D := A^T \Gamma^{-1/2}$, and $\xi_i = -\Gamma^{-1/2}(Au_i - y_i) \sim \mathcal{N}(0, I)$ and note that
\[ (A^T \Gamma^{-1} A + \lambda I)^{-1} A^T \Gamma^{-1} y_i - u_i = (DD^T + \lambda I)^{-1} A^T \Gamma^{-1} (Au_i + \xi_i) - u_i = (DD^T + \lambda I)^{-1} (\lambda u_i + D\xi_i). \]

Therefore we define
\[ f(\lambda, z) = \text{Tr}((DD^T + \lambda I)^{-2}(\lambda u + D\xi)(\lambda u + D\xi)^T) \]
\[ = \text{Tr}((DD^T + \lambda I)^{-2}(\lambda^2 uu^T + 2\lambda D\xi u^T + D\xi D^T)). \]

**A.2. Pointwise consistency analysis.** To apply Proposition 2.2, it is necessary to show the gradient of $\hat{F}_n(\lambda)$ is a good approximation of $\nabla F(\lambda)$ at $\lambda = \lambda_*$ with high probability. This is actually true for general $\lambda$.

To show this, we start by showing the sample covariance are consistent.

**Lemma A.1.** Let $X^{(i)}$ and $Y^{(i)}$ be i.i.d. $\mathcal{N}(0, I)$, $i \in \mathbb{N}$, let $\Sigma \in \mathbb{R}^{d \times d}$ be fixed. There exists a universal constant $c > 0$, such that for any $n$ and
\[ C_n = \frac{1}{n} \sum_{i=1}^{n} X^{(i)}(X^{(i)})^T, \quad B_n = \frac{1}{n} \sum_{i=1}^{n} X^{(i)}(Y^{(i)})^T, \]
the following holds
\[ \mathbb{P}(|\text{Tr}(\Sigma C_n) - \text{Tr}(\Sigma)| > t) \leq 2 \exp \left( -cn \min \left( \frac{t^2}{\|\Sigma\|^2 \|\Sigma\|^2}, \frac{t}{\|\Sigma\|^2 \|\Sigma\|^2} \right) \right), \]
\[ \mathbb{P}(|\text{Tr}(\Sigma B_n)| > t) \leq 2 \exp \left( -cn \min \left( \frac{t^2}{\|\Sigma\|^2 \|\Sigma\|^2}, \frac{t}{\|\Sigma\|^2 \|\Sigma\|^2} \right) \right). \]

**Proof.** First note
\[ \text{Tr}(\Sigma u_i u_i^T) = u_i^T \Sigma u_i. \]
We define the block-diagonal matrix $D_\Sigma \in \mathbb{R}^{nd \times nd}$ which consists of $n$ blocks of $\Sigma$, and $Z = [u_1; u_2; \cdots; u_n] \in \mathbb{R}^{nd}$. Note that
\[ \text{Tr}(\Sigma C_u) = Z^T (\frac{1}{n} D_\Sigma) Z. \]
By the Hanson–Wright inequality [42, Theorem 1.1], we obtain for some constants $c_0$ and $K$,
\[ \mathbb{P}(|\text{Tr}(\Sigma C_u) - \text{Tr}(\Sigma)| > t) \leq 2 \exp \left( -c_0 \min \left( \frac{t^2}{K^4 \|\frac{1}{n} D_\Sigma\|^2 \|\Sigma\|^2}, \frac{t}{K^2 \|\frac{1}{n} D_\Sigma\|^2} \right) \right). \]
Note that
\[ \|\frac{1}{n} D_\Sigma\|^2 = \frac{1}{n^2} \|D_\Sigma\|^2 = \frac{1}{n} \|\Sigma\|^2. \]
Consider then a block-diagonal matrix 

$$D = \begin{pmatrix} Y & 0 \\ 0 & Z \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

By the Hanson–Wright inequality $P(|\text{Tr}(\Sigma B)| > t) \leq 2 \exp\left(-c \min\left(\frac{t^2}{K^4\|\Sigma\|^2}, \frac{t}{K^2\|\Sigma\|}\right)\right)$.

We compute

$$\partial f(\lambda, z) = \text{Tr}\left(-2Q^2_1(\lambda^2 uu^T + 2\lambda D\xi u^T + D\xi^T D^T) + Q^4_1(2\lambda uu^T + 2D\xi u^T)\right).$$

$$\partial^2 f(\lambda, z) = 2\text{Tr}\left(3(DD^T + \lambda I)^{-4}(\lambda^2 uu^T + 2\lambda D\xi u^T + D\xi^T D^T) \right.$$

$$\left. - 4(DD^T + \lambda I)^{-3}(\lambda uu^T + D\xi u^T) + (DD^T + \lambda I)^{-2} uu^T\right).$$

Consider then a block-diagonal matrix $DQ \in \mathbb{R}^{n \times n}$ which consists of $n$ blocks of $Q$, and $Z = [u_1; \xi_1; u_2; \xi_2; \cdots; \xi_n; u_n] \in \mathbb{R}^{n \times 3}$. Then we can verify that

$$\text{Tr}(\Sigma B) = Z^T (\frac{1}{n} DQ) Z.$$ 

By the previous result we obtain the following convergence results.

**Lemma A.2.** Let $Q_\lambda = (DD^T + \lambda I)^{-1}$, the empirical loss function $\hat{F}_n$ is $C^3$ in $\lambda$, and for any $\lambda \in (\lambda_1, \lambda_r)$, there exists constants $C, c > 0$ such that for all $\varepsilon > 0$

$$P(|\partial \lambda \hat{F}_n(\lambda) - 2(\lambda/\lambda_r - 1)\text{Tr}(Q^3_1)| > \varepsilon) \leq C \exp(\varepsilon c \min\{\varepsilon, \varepsilon^2\}),$$

and

$$P(|\partial^2 \lambda \hat{F}_n(\lambda) - \frac{1}{\lambda^2} \text{Tr}(3(DD^T + \lambda I)^{-4}(\lambda^2 uu^T + 2\lambda D\xi u^T + D\xi^T D^T))| > \varepsilon) \leq C \exp(-c \min\{\varepsilon, \varepsilon^2\}),$$

where we have defined $D := A^T \Gamma^{-1/2}$ and $Q_\lambda = (DD^T + \lambda I)^{-1}$.

**Proof.** We compute

$$\partial \lambda f(\lambda, z) = \text{Tr}\left(-2Q^2_1(\lambda^2 uu^T + 2\lambda D\xi u^T + D\xi^T D^T) + Q^4_1(2\lambda uu^T + 2D\xi u^T)\right).$$

$$\partial^2 \lambda f(\lambda, z) = 2\text{Tr}\left(3(DD^T + \lambda I)^{-4}(\lambda^2 uu^T + 2\lambda D\xi u^T + D\xi^T D^T) \right.$$

$$\left. - 4(DD^T + \lambda I)^{-3}(\lambda uu^T + D\xi u^T) + (DD^T + \lambda I)^{-2} uu^T\right).$$

Since $\hat{F}_n(\lambda) = \frac{1}{n} \sum_{i=1}^n f(\lambda, 0)$, if we let

$$C_u = \frac{1}{n} \sum_{i=1}^n u_i u_i^T, \quad B = \frac{1}{n} \sum_{i=1}^n \xi_i u_i^T, \quad C_{\xi} = \frac{1}{n} \sum_{i=1}^n \xi_i \xi_i^T,$$
then
\[
\partial_\lambda \hat{F}_n(\lambda) = \text{Tr} \left( -2Q_\lambda^2 (\lambda^2 C_u + 2\lambda DB + DC_\xi D^\top) + Q_\lambda^2 (2\lambda C_u + 2DB) \right)
\]
(A.1)
\[
= -2\lambda^2 \text{Tr}(Q_\lambda^2 C_u) - 4\lambda \text{Tr}(Q_\lambda^3 DB) - 2\lambda \text{Tr}(D^\top Q_\lambda^3 DC_\xi) + 2\lambda \text{Tr}(Q_\lambda^3 C_u) \\
+ 2\text{Tr}(Q_\lambda^2 DB),
\]
and
\[
\partial_\lambda^2 \hat{F}_n(\lambda) = 2\text{Tr} \left( (3\lambda^2 Q_\lambda^4 - 4\lambda Q_\lambda^4 + Q_\lambda^2)C_u + 2(3\lambda Q_\lambda^4 - 2Q_\lambda^3)DB + 3Q_\lambda^4 DC_\xi D^\top \right)
\]
(A.2)
\[
= 2\text{Tr} \left( (3\lambda^2 Q_\lambda^4 - 4\lambda Q_\lambda^4 + Q_\lambda^2)C_u \right) - 8\lambda \text{Tr}(Q_\lambda^3 C_u) + 6\lambda \text{Tr}(Q_\lambda^3 DB) \\
- 4\text{Tr}(Q_\lambda^3 DB) + 6\text{Tr}(D^\top Q_\lambda^3 DC_\xi).
\]
Therefore
\[
\partial_\lambda^2 \hat{F}_n(\lambda) = 2\text{Tr} \left( (3\lambda^2 Q_\lambda^4 - 4\lambda Q_\lambda^4 + Q_\lambda^2)C_u + 2(3\lambda Q_\lambda^4 - 2Q_\lambda^3)DB + 3Q_\lambda^4 DC_\xi D^\top \right)
\]
(A.3)
\[
= 2\text{Tr} \left( (6\lambda Q_\lambda^4 - 12\lambda^2 Q_\lambda^3 + 4Q_\lambda^3 + 12\lambda Q_\lambda^4 - 2Q_\lambda^3)C_u \\
+ 2(3Q_\lambda^4 - 12\lambda Q_\lambda^3 + 6Q_\lambda^4)DB - 12Q_\lambda^4 DC_\xi D^\top \right).
\]

We note that \(\|Q_\lambda\| \leq \frac{1}{\lambda} \leq \frac{1}{\lambda_\tau}\) for all \(\lambda \geq \lambda_\tau\) and \(\|Q_\lambda\|^2 \leq \frac{d}{\lambda^2}\) respectively, and that
\[
\mathbb{E}\partial_\lambda \hat{F}_n(\lambda) = 2(\lambda/\lambda_u - 1)\text{Tr}(Q_\lambda^3),
\]
where the expectation is averaging realizations of \(\zeta\). Moreover, in (A.1), \(\partial_\lambda \hat{F}_n\) can be written as sum of \(\text{Tr}(\Sigma C_u), \text{Tr}(\Sigma B)\) and \(\text{Tr}(\Sigma C_\xi)\) for certain matrices \(\Sigma\). Note that for any random variables \(A_k\)
\[
\mathbb{P} \left( \sum_{k=1}^{m} (A_k - \mathbb{E}A_k) > \varepsilon \right) \leq \sum_{k=1}^{m} \mathbb{P}(|A_k - \mathbb{E}A_k| > \epsilon/m).
\]
Therefore we can apply Lemma A.1 at each trace term, and bound its probability of deviating from its mean. Therefore, we can find constants \(C_1, c\) such that
\[
\mathbb{P}(\partial_\lambda \hat{F}_n(\lambda) - 2(\lambda/\lambda_u - 1)\text{Tr}(Q_\lambda^3)) > \varepsilon \leq C_1 \exp \left( -cn \min(\varepsilon^2, \varepsilon) \right).
\]

We can apply the similar method to show the second assertion, since
\[
\mathbb{E}\partial_\lambda^2 \hat{F}_n(\lambda) = \frac{2}{\lambda^2} \text{Tr} \left( (3\lambda I - 2\lambda I + DD^\top)DD^\top Q_\lambda^3 \right).
\]

\[\square\]

**Remark A.3.** It is worthwhile to note that
\[
\partial_\lambda^2 F(\lambda) = \mathbb{E}\partial_\lambda^2 \hat{F}_n(\lambda) = \frac{2}{\lambda^2} \text{Tr} \left( (3\lambda I - 2\lambda I + DD^\top)DD^\top Q_\lambda^3 \right)
\]
is not always positive, and it can be negative if \(\lambda\) is very large. In other words, \(F\) is not convex on the real line. Therefore, it is necessary to introduce a local parameter domain where \(F\) is convex inside.

**Remark A.4.** We note that through the definition of \(f\), we can ensure that
\[
\mathbb{E}[\partial_\lambda f(\lambda, z)] = \partial_\lambda \mathbb{E}[f(\lambda, z)].
\]
This can be seen, by the following computation of \(\mathbb{E}[f(\lambda, z)]\). We can write
\[
\mathbb{E}[f(\lambda, z)] = \|Q_\lambda^{-1}(\lambda u + D\xi)\|^2 \\
= \text{Tr} \left( \text{Cov}(Q_\lambda^{-1}(\lambda u + D\xi), Q_\lambda^{-1}(\lambda u + D\xi)) \right).
\]
and with

\[ Q_\lambda^{-1}(\lambda u + D\xi) \sim \mathcal{N}(0, Q_\lambda^{-1}(\lambda^2 I + D\Gamma D^\top)Q_\lambda^{-1}) \]

we obtain

\[ \mathbb{E}[f(\lambda, z)] = \text{Tr}(Q_\lambda^{-1}(\lambda^2 I + D\Gamma D^\top)Q_\lambda^{-1}) \]
\[ = \text{Tr}(Q_\lambda^{-2}(\lambda^2 I + D\Gamma D^\top)). \]

Hence, we imply

\[ \partial_\lambda \mathbb{E}[f(\lambda, z)] = \text{Tr}(-2Q_\lambda^2(\lambda^2 I + D\Gamma D^\top) + 2Q_\lambda^2 \lambda). \]

A.3. **Consistency analysis within an interval.** To apply Proposition 2.2, it is also necessary to show the \( \hat{F}_n(\lambda) \) is strongly convex in a local region/interval. This can be done using a chaining argument in probability theory.

First, we show that the empirical loss function has bounded derivatives with high probability.

**Lemma A.5.** There exists an \( L > 0 \) such that the following holds true

\[ \mathbb{P} \left( \max_{\lambda_i \in \mathcal{A}_n} |\partial_k^k \hat{F}_n(\lambda)| > L, k = 1, 2, 3 \right) \leq 6 \exp(-nc). \]

**Proof.** Recall that \( \|Q_\lambda\| \leq \frac{1}{\lambda} \) and the formulae (A.1), (A.2) and (A.3). It is easy to see that if \( C_u, B, C_\xi \) are all bounded in operator norm, then \( |\partial_k^k \hat{F}_n(\lambda)| \) will be uniformly bounded for all \( M^{-1} \leq \lambda \leq M \). While if we take \( t = \sqrt{d} \) in Lemma A.1

\[ \mathbb{P}(|C_u| > d\lambda^{-1} + \sqrt{d}) \leq \mathbb{P}(\text{Tr}(C_u) > d\lambda^{-1} + \sqrt{d}) \]
\[ \leq 2 \exp(-cn \min(d/d, \sqrt{d})) = 2 \exp(-cn), \]

\[ \mathbb{P}(|C_\xi| > d + \sqrt{d}) \leq \mathbb{P}(\text{Tr}(C_\xi) > d + \sqrt{d}) \leq 2 \exp(-cn), \]
\[ \mathbb{P}(|B| > d + \sqrt{d}) \leq \mathbb{P}(\text{Tr}(B) > d + \sqrt{d}) \leq 2 \exp(-cn). \]

Then with certain constants \( M(\lambda) \) and \( \lambda = M(\lambda)(d\lambda^{-1} + d + \sqrt{d}) \)

\[ \mathbb{P} \left( \max_{M^{-1} \leq \lambda \leq M} |\partial_k^k \hat{F}_n(\lambda)| \leq L_M, k = 1, 2, 3 \right) \]
\[ \geq \mathbb{P} \left( |C_u| \leq d\lambda^{-1} + \sqrt{d}, |C_\xi| \leq d + \sqrt{d}, |B| \leq d + \sqrt{d} \right) \]
\[ \geq 1 - 6 \exp(-nc). \]

Next, we show that if \( f(n) \) is bounded at each fixed point with high probability, it is likely to be bounded on a fixed interval if it is Lipschitz.

**Lemma A.6.** Let \( f_n(\lambda) \) be function of \( \lambda \) and the following is true for some interval \( I = [\lambda_l, \lambda_u] \)

\[ \mathbb{P}(f_n(\lambda) > a) \leq C \exp(-ncu) \quad \forall \lambda_l \leq \lambda \leq \lambda_u. \]

Then

\[ \mathbb{P} \left( \max_{\lambda \in I} f_n(\lambda) > 2a, \max_{\lambda \in I} |\partial f_n(\lambda)| \leq M \right) \leq a^{-1}|\lambda_u - \lambda_l|MC \exp(-ncu). \]

Let \( f_n(\lambda) \) be function of \( \lambda \) and the following is true for some interval \( I \)

\[ \mathbb{P}(f_n(\lambda) < a) \leq \exp(-ncu) \quad \forall \lambda_l \leq \lambda \leq \lambda_u. \]

Then

\[ \mathbb{P} \left( \min_{\lambda \in I} f_n(\lambda) < a/2, \max_{\lambda \in I} |\partial f_n(\lambda)| \leq M \right) \leq 2a^{-1}|\lambda_u - \lambda_l|MC \exp(-ncu). \]
Proof. Pick \( \lambda_i = \lambda + \frac{2a}{|M|} \) for \( i = 0, \ldots, \left\lfloor \frac{\lambda_n - \lambda}{2a} \right\rfloor \). Then \( \lambda_i \leq \lambda_i \leq \lambda_u \), and for any \( \lambda_i \leq \lambda \leq \lambda_i \), \( |\lambda - \lambda_i| \leq \frac{a}{M} \) for some \( \lambda_i \). Not that if \( |\partial f_n(\lambda)| \leq M \), and \( f_n(\lambda_i) \leq a \), for all \( i \), then for any \( \lambda_i \leq \lambda \leq \lambda_u \),

\[
f_n(\lambda) \leq f_n(\lambda_i) + (\lambda_i - \lambda)\partial f_n(\lambda) \leq a + \frac{a}{M}M = 2a.
\]

Consequently, by union bound

\[
P\left( \min_{\lambda \in I} f_n(\lambda) > 2a, \max_{\lambda \in I} |\partial f_n(\lambda)| \leq M \right) \leq P\left( f_n(\lambda_i) > a \right. \text{ for some } i \right.
\]

\[
\leq a^{-1} |\lambda_u - \lambda_i|MC \exp(-nc_a).
\]

The same argument can be applied to show the second claim, except that we choose \( \lambda_i = c + \frac{a}{|M|} \).

\[\square\]

The next lemma indicates that the loss function is strongly convex within \( D \) with high probability.

**Lemma A.7.** Assume that the largest eigenvalue of \( DD^T \) is \( \lambda_D \) and let \( \lambda \in D := \left[ \frac{1}{2} \lambda_u, \frac{3}{2} \lambda_u \right] \). Then for some constants \( c, C > 0 \),

\[
P(\min_{\lambda \in D} \partial^2_{\lambda} \hat{F}_n(\lambda) < H_*/4) \leq \frac{C}{\min \{ H_*, 1 \}} \exp\left( -cn \min(\lambda_D^2, H_*, 1) \right),
\]

with

\[
H_* = H_*(\lambda_D, \lambda_u) = \frac{2\lambda_D^2}{(\lambda_D + \lambda)^2 \lambda_u} > 0.
\]

**Proof.** Note that for any \( \lambda \in D \), and \( v \) being the eigenvector of \( DD^T \) corresponds to the largest eigenvalue \( \lambda_D \),

\[
\frac{2}{\lambda_u} \text{Tr} ((3\lambda I - 2M + DD^T)DD^TQ_\lambda^4) \geq \frac{2}{\lambda_u} \text{Tr} (DD^TDD^TQ_\lambda^4)
\]

\[
\geq 2 \lambda_u \text{Tr} (v^TDD^TDD^TQ_\lambda^4v)
\]

\[
= \frac{2\lambda_D^2}{(\lambda_D + \lambda)^2 \lambda_u} \geq H_*
\]

for \( \lambda \in D \) and we set \( \varepsilon = H_*/2 > 0 \) to apply Corollary A.2. We obtain some \( C_1, c_1 \)

\[
C_1 \exp\left( -cn \min(\lambda_D^2, H_*) \right)
\]

\[
\geq P\left( \partial^2_{\lambda} \hat{F}_n(\lambda) - \frac{2}{\lambda_u} \text{Tr} ((3\lambda I - 2M + DD^T)DD^TQ_\lambda^4) > H_*/2 \right)
\]

\[
\geq P\left( \partial^2_{\lambda} \hat{F}_n(\lambda) < \frac{2}{\lambda_u} \text{Tr} ((3\lambda I - 2M + DD^T)DD^TQ_\lambda^4) - H_*/2 \right)
\]

\[
\geq P(\partial^2_{\lambda} \hat{F}_n(\lambda) < H_*/2).
\]

By Lemma A.5 there exists an \( L > 0 \) and \( c_1 \) such that

\[
P\left( \max_{\lambda \in D} |\partial^2_{\lambda} \hat{F}_n(\lambda)| > L \right) \leq 6 \exp(-nc_1),
\]

and by Lemma A.6 it holds true that

\[
\frac{C_2}{\min \{ H_*, 1 \}} \exp\left( -cn \min(\lambda_D^2, H_*) \right)
\]

\[
\geq P\left( \min_{\lambda \in D} \partial^2_{\lambda} \hat{F}_n(\lambda) < H_*/4, \max_{\lambda \in D} |\partial^2_{\lambda} \hat{F}_n(\lambda)| \leq M \right).
\]
for some $C_2 > 0$. We define the sets $A_n := \{\min_{\lambda \in D} \partial_3^2 \tilde{F}_n(\lambda) < H_*/4\}$ and $B_n := \{\max_{\lambda \in D} |\partial_3^2 \tilde{F}_n(\lambda)| \leq L\}$, and we obtain
\[
\mathbb{P}(\min_{\lambda \in D} \partial_3^2 \tilde{F}_n(\lambda) < H_*/4) = \mathbb{P}(A_n | B_n)\mathbb{P}(B_n) + \mathbb{P}(A_n | B_n^c)\mathbb{P}(B_n^c)
\leq \mathbb{P}(A_n \cap B_n) + \mathbb{P}(B_n^c)
\leq \frac{C}{\min(H_*/1)} \exp\left(-cn\min(H_*/1, 1)\right).
\]
\[\square\]

The last lemma indicates the empirical loss function is unlikely to have local minima outside $[\frac{1}{2} \lambda_*, \frac{3}{2} \lambda_*]$. 

**Lemma A.8.** Assume again that the largest eigenvalue of $DD^T$ is $\lambda_D$. Let $L_* = \frac{1}{(\lambda_D + \lambda_0)^2}$. There are constants $c, C$ such that
\[
\mathbb{P}\left(\min_{\lambda_* \geq \lambda > \frac{3}{2} \lambda_*} \partial_3 \tilde{F}_n(\lambda) < L_*/4\right) \leq \frac{C}{\min[\lambda_*, 1]} \exp\left(-cn\min\left(L_*, \frac{3}{2} \lambda_*\right)\right),
\]
and
\[
\mathbb{P}\left(\min_{\frac{1}{2} \lambda_* \geq \lambda > \lambda_*} \partial_3 \tilde{F}_n(\lambda) > -L_*/4\right) \leq \frac{C}{\min[\lambda_*, 1]} \exp\left(-cn\min\left(L_*, \frac{3}{2} \lambda_*\right)\right).
\]

**Proof.** We first note that with $v$ being the leading eigenvector of $DD^T$, 
\[
\text{Tr}(Q_3^3) \geq v^T Q_3^3 v \geq L_.*
\]
And for $\lambda > \frac{3}{2} \lambda_*$ we have
\[
2(\lambda/\lambda_* - 1)\text{Tr}(Q_3^3) \geq L_*.
\]
We set $\varepsilon = L_*/2$ to apply Lemma A.2 and obtain
\[
C \exp\left(-nc\min(L_*, \lambda_*)\right) \geq \mathbb{P}(|\partial_3 \tilde{F}_n(\lambda) - 2(\lambda/\lambda_* - 1)\text{Tr}(Q_3^3)| > L_*/2)
\geq \mathbb{P}(\partial_3 \tilde{F}_n(\lambda) < 2(\lambda/\lambda_* - 1)\text{Tr}(Q_3^3) - L_*/2).
\]
Similarly as in Lemma A.7, we use Lemma A.5 and Lemma A.6 to obtain the first assertion.

We obtain the second assertion by using
\[
2(\lambda/\lambda_* - 1)\text{Tr}(Q_3^3) \leq -L_* < 0,
\]
for $\lambda < \frac{1}{2} \lambda_*$. \[\square\]

**A.4. Summarizing argument.** Finally, we are ready to prove Theorem 2.3.

**Proof of Theorem 2.3.** Denote $D = [\frac{1}{2} \lambda_*, \frac{3}{2} \lambda_*], H_* = \frac{2\lambda_0^2}{(\lambda_D + 3\lambda_0/2)^2 \lambda_*}$ and the events 
\[
B = \{\lambda_l < \lambda_0 < \lambda_u\}, \quad A_n = \{\tilde{\lambda}_n \in D, \partial_3^2 \tilde{F}_n(\lambda) \geq \frac{1}{2} H_* \text{ for all } \lambda \in D\}.
\]
First we decompose
\[
\mathbb{P}(|\tilde{\lambda}_n - \lambda_*| > \varepsilon, B) = \mathbb{P}(|\tilde{\lambda}_n - \lambda_*| > \varepsilon, B \mid A_n) \cdot \mathbb{P}(A_n)
+ \mathbb{P}(|\tilde{\lambda}_n - \lambda_*| > \varepsilon, B \mid A_n^c) \cdot \mathbb{P}(A_n^c)
\leq \mathbb{P}(|\tilde{\lambda}_n - \lambda_*| > \varepsilon, B \mid A_n) + \mathbb{P}(B \cap A_n^c).
\]
In the last step we have used \( P(\hat{\lambda}_n \leq \lambda_u) = 1 \). By Proposition 2.2
\[
\mathbb{P}(|\hat{\lambda}_n - \lambda_*| > \epsilon, B \mid A_n) \leq \mathbb{P}\left( |\partial_\lambda \tilde{F}_n(\lambda_*) - \partial_\lambda F(\lambda_*)| > \frac{1}{4} H_* \epsilon, B \right)
\]
\[
= \mathbb{P}\left( |\partial_\lambda \tilde{F}_n(\lambda_*)| > \frac{1}{4} H_* \epsilon, B \right),
\]
which can be bounded by Lemmas A.2 and A.6
\[
\mathbb{P}(|\hat{\lambda}_n - \lambda_*| > \epsilon \mid A_n) \leq C_1 \exp(-nc_1 \min\{\epsilon, \epsilon^2\}),
\]
for some \( C_1, c_1 \).

We bound the probability \( \mathbb{P}(A_n^c) \) by
\[
\mathbb{P}(B \cap A_n^c) \leq \mathbb{P}(B, \hat{\lambda}_n \notin D) + \mathbb{P}(\{\partial_\lambda^2 \tilde{F}_n(\lambda) \geq H_*/4 \text{ for all } \lambda \in D\}^c),
\]
and study both terms separately. Note first, by Lemma A.8, for some constants \( C_2, c_2 > 0 \) the following holds
\[
\mathbb{P}(B, \hat{\lambda}_n \notin D) \leq \mathbb{P}(\partial_\lambda \tilde{F}_n(\lambda) = 0 \text{ for some } \lambda \in (\lambda_1, \lambda_u) \setminus D)
\]
\[
\leq C_2 \exp(-c_2 n).
\]
Second, by Lemma A.7, for some constants \( C_3, c_3 > 0 \) we obtain
\[
\mathbb{P}(\{\partial_\lambda^2 \tilde{F}_n(\lambda) \geq H_*/4 \text{ for all } \lambda \in D\}^c) \leq C_3 \exp(-c_3 n).
\]
Finally, there exist some constants \( C_*, c_* > 0 \) such that
\[
\mathbb{P}(|\hat{\lambda}_n - \lambda_*| > \epsilon) \leq C_* \exp(-c_* n \min(\epsilon, \epsilon^2)).
\]
\( \square \)

Appendix B. Online consistency analysis

B.1. Stochastic gradient decent. We start by verifying Lemma 3.2.

Proof of Lemma 3.2. We apply the implicit function theorem to prove this statement. For fixed \( y \in \mathbb{R}^K \), we define the function
\[
\varphi(\lambda, u) := \nabla_u \Psi(\lambda, u, y).
\]
Since \( (\lambda, u) \mapsto \Psi(\lambda, u, y) \) is strictly convex, we have that for all \( (\lambda, u) \) near \( (\lambda_0, u_{\lambda_0}) \) the Jacobian of \( \varphi \) w.r.t. \( u \) is invertible, i.e.
\[
D_u \varphi(\lambda, u) = \nabla_u^2 \Psi(\lambda, u, y) > 0.
\]

Set \( \bar{\lambda} \in \mathbb{R}^d \) arbitrary, then for \( \bar{u} = u_{\bar{\lambda}}(y) \) it holds true that
\[
\varphi(\bar{\lambda}, \bar{u}) = 0
\]
and by the implicit function theorem there exists a open neighborhood \( D \subset \mathbb{R}^d \) of \( \lambda_0 \) with \( \bar{\lambda} \in D \) such that there exists a unique continuously differentiable function \( \bar{U} : D \rightarrow \mathbb{R}^d \) with \( \bar{U}(\bar{\lambda}) = \bar{u} \) and
\[
\varphi(\lambda, \bar{U}(\lambda)) = 0,
\]
for all \( \lambda \in \Lambda \), i.e. \( \bar{U} \) maps all \( \lambda \in \Lambda \) to the corresponding regularized solution \( \bar{U}(\lambda) = u_{\lambda}(y) \). Further, the partial derivatives of \( \bar{U} \) are given by
\[
\frac{\partial \bar{U}}{\partial \lambda_i}(\lambda) = -\left[D_u \varphi(\lambda, \bar{U}(\lambda))\right]^{-1} \left[\frac{\partial \varphi}{\partial \lambda_i}(\lambda, \bar{U}(\lambda))\right].
\]
Since the choice of \( \lambda \in \mathbb{R}^d \) is arbitrary, it follows that \( \lambda \mapsto u_{\lambda}(y) \) is continuously differentiable with derivative given by
\[
\nabla_{\lambda} u_{\lambda}(y) = -\left(\nabla_u^2 \Psi(\lambda, u_{\lambda}(y), y)\right)^{-1} \nabla_u^2 \Psi(\lambda, u_{\lambda}(y), y).
\]
The computation of \( \nabla_{\lambda} f \) can be obtained by the chain rule.
B.2. General consistency analysis framework.

Proof of Proposition 3.3. Note that
\[
\Delta_{k+1} = \chi(\lambda_k - \beta_k \nabla \lambda f(\lambda_k, Z_k)) - \lambda_* ,
\]
and apply Lemma 3.1
\[
\|\Delta_{k+1}\|^2 = \|\chi(\lambda_k - \beta_k \nabla \lambda f(\lambda_k, Z_k)) - \lambda_*\|^2 \leq \|\lambda_k - \beta_k \nabla \lambda f(\lambda_k, Z_k) - \lambda_*\|^2 \\
= \|\Delta_k - \beta_k \nabla \lambda f(\lambda_k, Z_k)\|^2 \\
= \|\Delta_k - \beta_k \nabla \lambda F(\lambda_k, Z_k) - \beta_k \delta_k - \beta_k \xi_k\|^2,
\]
where
\[
\delta_k = \mathbb{E}_k \nabla f(\lambda_k, Z) - \nabla F(\lambda_k), \quad \xi_k = \nabla \lambda f(\lambda_k, Z_k) - \mathbb{E}_k \nabla \lambda f(\lambda_k, Z)
\]
is the bias and noise in the stochastic gradient, we denote the expectation conditioned on information available at step \( k \) as \( \mathbb{E}_k \) and define the first exit time of \( \mathcal{D} \) by with \( \tau = \inf\{ k \geq 0 | \lambda_k \in \mathcal{D} \} \). Next, we note that
\[
\mathbb{E}_k \| \nabla f(\lambda_k, Z_k) \|^2 = \| \nabla \lambda F(\lambda_k) + \delta_k \|^2 + \mathbb{E}_k \| \xi_k \|^2.
\]
So if \( \tau \geq k \),
\[
\mathbb{E}_k \| \Delta_{k+1} \|^2 \leq \| \Delta_k \|^2 - 2 \beta_k \Delta_k^T (\nabla \lambda F(\lambda_k) + \delta_k) + \beta_k^2 \| \nabla \lambda F(\lambda_k) + \delta_k \|^2 + \mathbb{E}_k \| \xi_k \|^2 \\
\leq \| \Delta_k \|^2 - 2 \beta_k \Delta_k^T \nabla \lambda F(\lambda_k) + 2 \beta_k \| \Delta_k \| \| \delta_k \| + \beta_k^2 (a + b \| \Delta_k \|^2) \\
\leq \| \Delta_k \|^2 - 2 c \beta_k \| \Delta_k \| \| \delta_k \| + \frac{1}{2} \beta_k \| \Delta_k \| ^2 + \frac{2}{c} \beta_k \| \delta_k \| ^2 + \beta_k^2 a + b \beta_k^2 \| \Delta_k \| ^2 \\
\leq (1 - 1.5 c \beta_k + b \beta_k^2) \| \Delta_k \| ^2 + (a \beta_k + 2 a \beta_k/c) \beta_k.
\]
Since \( \beta_k < c/2b \), we have
\[
\mathbb{E}_k 1_{\tau \geq k+1} \| \Delta_{k+1} \|^2 \leq \mathbb{E}_k 1_{\tau \geq k} \| \Delta_{k+1} \|^2 \leq 1_{\tau \geq k} (1 - c \beta_k) \| \Delta_k \|^2 + (a \beta_k + 2 a \beta_k/c) \beta_k.
\]
Let \( Q_k = 1_{\tau \geq k} \| \Delta_k \|^2 \), then we just derived that
\[
\mathbb{E}_k Q_{k+1} \leq (1 - c \beta_k) \mathbb{E} Q_k + (a \beta_k + 2 a \beta_k/c) \beta_k.
\]
Therefore by Gronwall’s inequality (B.1)
\[
\mathbb{E} Q_n \leq a \sum_{k=1}^n \left( \prod_{j=k+1}^n (1 - c \beta_j) \beta_k^2 \right) + \frac{2}{c} \sum_{k=1}^n \left( \prod_{j=k+1}^n (1 - c \beta_j) \beta_k \right) + \exp \left( -c \sum_{j=1}^n \beta_j \right) \mathbb{E} Q_0.
\]
Next we look at the 2nd term of (B.1). Note that when \( a \beta_k \leq a_0 \), then
\[
\frac{2}{c} \sum_{k=1}^n \prod_{j=k+1}^n (1 - c \beta_j) \beta_k \leq \frac{a_0}{c} \sum_{k=1}^n \prod_{j=k+1}^n (1 - c \beta_j) c \beta_k \\
\leq \frac{a_0}{c} \sum_{k=1}^n \left( \prod_{j=k+1}^n (1 - c \beta_j) - \prod_{j=k}^n (1 - c \beta_j) \right) \leq \frac{a_0}{c^2}.
\]
In this case, (B.1) becomes
\[
\mathbb{E} Q_n \leq a \sum_{k=1}^n \left( \prod_{j=k+1}^n (1 - c \beta_j) \beta_k^2 \right) + \frac{a_0}{c^2} + \exp \left( -c \sum_{j=1}^n \beta_j \right) \mathbb{E} Q_0.
\]
And if $\alpha_k \leq D\beta_k$, then (B.1) can be simplified as

$$E Q_n \leq (a + D/c) \sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) \beta_k^2 \right) + \exp \left( -c \sum_{j=1}^{n} \beta_j \right) EQ_0.$$ 

In both cases, to show our claim, we just need to show

$$\sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) \beta_k^2 \right) \leq 2C_n, \quad \exp \left( -c \sum_{j=1}^{n} \beta_j \right) \leq C_n.$$ 

Let $k_0$ be the minimizer of

$$k_0 = \arg \min_{k \leq n} \max \{ \prod_{j=k+1}^{n} (1 - c\beta_j), a\beta_k/c \}$$

Then note that,

$$\sum_{k=1}^{k_0} \prod_{j=k+1}^{n} (1 - c\beta_j) \beta_k^2 \leq \sum_{k=1}^{k_0} \prod_{j=k+1}^{n} (1 - c\beta_j) \beta_k^2 \leq \prod_{j=1}^{k_0} (1 - c\beta_j) \sum_{k=1}^{\infty} \beta_k^2 \leq C_n.$$ 

also

$$\sum_{k=k_0+1}^{n} \prod_{j=k+1}^{n} (1 - c\beta_j) \beta_k^2 \leq \frac{1}{c} \beta_{k_0} \sum_{k=1}^{k_0} \prod_{j=k+1}^{n} (1 - c\beta_j) c\beta_k \leq \frac{1}{c} \beta_{k_0} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) - \prod_{j=k}^{n} (1 - c\beta_j) \right) \leq \frac{1}{c} \beta_{k_0} = C_n.$$ 

The sum of the previous two inequalities leads to

$$\sum_{k=1}^{n} \left( \prod_{j=k+1}^{n} (1 - c\beta_j) \beta_k^2 \right) \leq 2C_n.$$ 

Finally

$$\exp(-c \sum_{j=1}^{n} \beta_j) EQ_0 \leq \exp(-c \sum_{j=k_0+1}^{n} \beta_j) EQ_0 \leq C_n.$$ 

To see that $C_n$ converges to zero, simply let

$$k_n = \max_k \left\{ k \left( \prod_{j=1}^{k} (1 - c\beta_j) > \prod_{j=1}^{n} (1 - c\beta_j) \right) \right\}$$

Because $\prod_{j=1}^{n} (1 - c\beta_j)$ decays to zero when $n \to \infty$, so $k_n$ will increases to $\infty$, and $\beta_{k_n}$ will decay to zero. Meanwhile,

$$C_n \leq \min \left\{ \prod_{j=k+1}^{n} (1 - c\beta_j), \beta_{k_n} \right\} \leq \min \left\{ \prod_{j=1}^{n} (1 - c\beta_j), \beta_{k_n} \right\},$$

which will decay to zero when $n \to \infty$. □
B.3. Application to linear inverse problems.

Proof of Theorem 3.5. We will set $D = \Lambda = [\lambda_1, \lambda_n]$. Then because $\chi$ always bring $\lambda_k$ back into $D$, the event $\mathcal{A}$ always happen.

We have seen in the proof of Lemma A.8, that

$$\nabla_\Lambda F(\lambda) = 2(\Lambda/\lambda_\star - 1)\text{Tr}(Q_\lambda^2 D^T D).$$

Multiplication with $(\lambda - \lambda_\star)$ gives

$$(\lambda - \lambda_\star)\nabla_\Lambda F(\lambda) = 2(\lambda - \lambda_\star)^2\text{Tr}(Q_\lambda^2 D^T D / \lambda_\star).$$

So if we take

$$c = 2\text{Tr}(Q_\lambda^2 D^T / \lambda_\star) > 0$$

(3.7) is verified.

To show (3.9), we will prove

$$E[\widetilde{\nabla}_\Lambda f(\lambda, Z) - \nabla_\Lambda f(\lambda, Z)]^2 = E[\nabla_\Lambda f(\lambda, Z) - \nabla_\Lambda f(\lambda, Z)]^2 \quad \leq E(\nabla_\Lambda f(\lambda, Z) - \nabla_\Lambda f(\lambda, Z))^2.$$

First note that it holds true that

$$E[||u_\lambda(y) - u||^4] \leq 8E[||u_\lambda(y)||^4] + 8E[||u||^4]$$

$$\leq 8(\|Q_\lambda\|^4(\|DD^T\|^4E[||u||^4] + E[||D\xi\|^4]) + 8E[u^4]$$

$$\leq 8(\|DD^T\|^2/\lambda_\star^4 + 1) m_2^4 + 8/\lambda_\star^4 m_4^2 := C_1.$$

Next, we show that

$$E[||\nabla_\Lambda u_\lambda(y) - \widetilde{\nabla}_\Lambda u_\lambda(y)||^4] \leq C_2 h^8.$$  

To this end, we apply Taylor series expansion of $u_\lambda(y) = Q_\lambda D^T (Du + \xi) = \varphi(\lambda) V$, with $V \sim N(0, D(1/\lambda^* D^T D + I)D^T)$ and $\varphi(\lambda) := Q_\lambda$, i.e. there exists $\lambda_+, \lambda_- \in [\lambda - h, \lambda + h]$ such that

$$\widetilde{\nabla}_\Lambda u_\lambda(y) - \nabla_\Lambda u_\lambda(y) = \frac{1}{12} \left( \varphi^{(3)}(\lambda_+) + \varphi^{(3)}(\lambda_-) \right) h^2 V.$$

Using $\varphi^{(k)}(\lambda) = (-1)^k Q^k_\lambda$, we can bound

$$E[||\frac{1}{12} \varphi^{(3)}(\lambda) h^2 V||^4] \leq \frac{1}{12^4 \lambda_\star^{10}} E[||V||^4] h^8,$$

for $\lambda \in [\lambda_1, \lambda_\star \lambda_- \in [\lambda_1, \lambda_\star]$ and we obtain (B.2) with $C_2 = 2/(12^4 \lambda_\star^{10}) E[||V||^4]$. Taking the square root finally verifies (3.9) with $\alpha_0 \in \mathcal{O}(h^4)$.

To prove that (3.8) is satisfied, we first compute

$$|\nabla_\Lambda f(\lambda, Z)|^2 = 2\lambda^2 \langle u, Q_\lambda^2 u \rangle - 4\lambda \langle u, Q_\lambda^2 D\xi \rangle - 2\langle D\xi, Q_\lambda^2 D\xi \rangle + 2\lambda \langle u, Q_\lambda^2 u \rangle$$

$$+ 2\langle u, Q_\lambda^2 D\xi \rangle^2 \leq 20\lambda^2 ||u||^2 ||Q_\lambda^2||^2 + 20\lambda^2 ||Q_\lambda^2||^2 ||u||^2 ||D\xi||^2 + 20\lambda^2 ||Q_\lambda^2||^2 ||u||^2 ||D\xi||^2 + 20\lambda^2 ||Q_\lambda^2||^2 ||u||^2 ||D\xi||^2 + 20\lambda^2 ||Q_\lambda^2||^2 ||u||^2 ||D\xi||^2 + 20\lambda^2 ||Q_\lambda^2||^2 ||u||^2 ||D\xi||^2.$$

We apply the bound

$$||Q_\lambda|| \leq \frac{1}{\lambda} \leq \frac{1}{\lambda_\star}, \quad \lambda \in \mathcal{D}$$
and obtain
\[ |\nabla \lambda f(\lambda, Z)|^2 \leq \frac{20}{\lambda^4} ||u||^4 + \frac{80}{\lambda^2} ||u||^2 ||D\xi||^2 + \frac{20}{\lambda^2} ||D\xi||^4 + \frac{20}{\lambda^2} ||u||^2 ||D\xi||^2. \]

Then we note that
\[ E[|\hat{\nabla} f(\lambda, Z)|^2] \leq 2E[|\nabla f(\lambda, Z)|^2] + 2E[|\nabla f(\lambda, Z) - \hat{\nabla} f(\lambda, Z)|^2] \]

Therefore, (3.8) holds with
\[ a = \frac{80}{\lambda^4} m_2^u + \frac{160}{\lambda^2} m_2^y + \frac{40}{\lambda^4} m_4^{D\xi} + \frac{40}{\lambda^2} m_2^u m_2^{D\xi} + \sqrt{C_1 C_2} h^4, \quad b = 0, \]

where \( m_2^u = E[||u||^2], \ m_2^y = E[||u||^4], \ m_4^{D\xi} = E[||D\xi||^2], \ m_2^{D\xi} = E[||D\xi||^4]. \)

\[ \square \]

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