

1 **L_p REGULARIZATION FOR ENSEMBLE KALMAN INVERSION***

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3 **Abstract.** Ensemble Kalman inversion (EKI) is a derivative-free optimization method that
4 lies between the deterministic and the probabilistic approaches for inverse problems. EKI iterates
5 the Kalman update of ensemble-based Kalman filters, whose ensemble converges to a minimizer
6 of an objective function. EKI regularizes ill-posed problems by restricting the ensemble to the
7 linear span of the initial ensemble, or by iterating regularization with early stopping. Another
8 regularization approach for EKI, Tikhonov EKI, penalizes the objective function using the l_2 penalty
9 term, preventing overfitting in the standard EKI. This paper proposes a strategy to implement l_p , $0 < p \leq 1$,
10 regularization for EKI to recover sparse structures in the solution. The strategy transforms a l_p
11 problem into a l_2 problem, which is then solved by Tikhonov EKI. The transformation is explicit, and
12 thus the proposed approach has a computational cost comparable to Tikhonov EKI. We validate the
13 proposed approach's effectiveness and robustness through a suite of numerical experiments, including
14 compressive sensing and subsurface flow inverse problems.

15 **Key words.** inverse problems, ensemble Kalman inversion, regularization, sparsity

16 **AMS subject classifications.** 65J20, 65C05, 35Q93, 49M41

17 **1. Introduction.** A wide range of problems in science and engineering are for-
18 mulated as inverse problems. Inverse problems aim to estimate a quantity of interest
19 from noisy, imperfect observation or measurement data, such as state variables or
20 a set of parameters that constitute a forward model. Examples include deblurring
21 and denoising in image processing [15], recovery of permeability in subsurface flow
22 using pressure fields [27], and training a neural network in machine learning [16, 23]
23 to name a few. In this paper, we consider the inverse problem of finding $u \in \mathbb{R}^N$ from
24 measurement data $y \in \mathbb{R}^m$ where u and y are related as follows

25 (1.1)
$$y = G(u) + \eta.$$

26 Here $G : \mathbb{R}^N \rightarrow \mathbb{R}^m$ is a forward model that can be nonlinear and computationally
27 expensive to solve, for example, solving a PDE problem. The last term η is a mea-
28 surement error. The measurement error is unknown in general, but we assume that
29 it is drawn from a known probability distribution, a Gaussian distribution with mean
30 zero and a known covariance Γ . By assuming that the forward model G and the
31 observation covariance Γ are known, the unknown variable u is estimated by solving
32 an optimization problem

33 (1.2)
$$\operatorname{argmin}_{u \in \mathbb{R}^N} \frac{1}{2} \|y - G(u)\|_{\Gamma}^2,$$

34 where $\|\cdot\|_{\Gamma}$ is the norm induced from the inner product using the inverse of the
35 covariance matrix Γ , that is $\|a\|_{\Gamma}^2 = \langle a, \Gamma^{-1}a \rangle$ for the standard inner product $\langle \cdot, \cdot \rangle$ in
36 \mathbb{R}^m .

37 Ensemble Kalman inversion (EKI), pioneered in the oil industry [27] and math-
38 ematically formulated in an application-neutral setting in [20], is a derivative-free
39 method that lies between the deterministic and the probabilistic approaches for in-
40 verse problems. EKI's key feature is an iterative application of the Kalman update

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41 of the ensemble-based Kalman filters [1, 13]. Ensemble-based Kalman filters are well
 42 known for their success in numerical weather prediction, stringent inverse problems
 43 involving high-dimensional systems. EKI iterates the ensemble-based Kalman update
 44 in which the ensemble mean converges to the solution of the optimization problem
 45 (1.2). EKI can be thought of as a least-squares method in which the derivatives are
 46 approximated from an empirical correlation of an ensemble [6], not from a variational
 47 approach. Thus, EKI is highly parallelizable without calculating the derivatives re-
 48 lated to the forward or the adjoint problem used in the gradient-based methods.

49 Inverse problems are often ill-posed, which suffer from non-uniqueness of the
 50 solution and lack stability. Also, in the context of regression, the solution can show
 51 overfitting. A common strategy to overcome ill-posed problems is regularizing the
 52 solution of the optimization problem [3]. That is, a special structure of the solution
 53 from prior information, such as sparsity, is imposed to address ill-posedness. The
 54 standard EKI [20] implements regularization by restricting the ensemble to the linear
 55 span of the initial ensemble reflecting prior information. The ensemble-based Kalman
 56 update is known for that the ensemble remains in the linear span of the initial ensemble
 57 [25, 20]. Thus, the EKI ensemble always stays in the linear span of the initial ensemble,
 58 which regularizes the solution. Although this approach shows robust results in certain
 59 applications, numerical evidence demonstrates that overfitting may still occur [20]. As
 60 an effort to address the overfitting of the standard EKI, an iterative regularization
 61 method has been proposed in [21], which approximates the regularizing Levenberg-
 62 Marquardt scheme [18]. As another regularization approach using a penalty term to
 63 the objective function, a recent work called Tikhonov EKI (TEKI) [9] implements the
 64 Tikhonov regularization (which imposes a l_2 penalty term to the objective function)
 65 using an augmented measurement model that adds artificial measurements to the
 66 original measurement. TEKI's implementation is a straightforward modification of
 67 the standard EKI method with a marginal increase in the computational cost.

68 The regularization methods for EKI mentioned above address several issues of
 69 ill-posed problems, including overfitting. However, it is still an open problem to
 70 implement other types of regularizers, such as l_1 or total variation (TV) regularization.
 71 This paper aims to implement l_p , $0 < p \leq 1$, regularization to recover sparse structures
 72 in the solution of inverse problems. In other words, we propose a highly-parallelizable
 73 derivative-free method that solves the following l_p regularized optimization problem

$$74 \quad (1.3) \quad \underset{u \in X}{\operatorname{argmin}} \frac{\lambda}{2} \|u\|_p^p + \frac{1}{2} \|y - G(u)\|_{\Gamma}^2,$$

75 where $\|u\|_p$ is the l_p norm of u , i.e., $\sum_i^N |u_i|^p$, and λ is a regularization coefficient.

76 The proposed method's key idea is a transformation of variables that converts
 77 the l_p regularization problem to the Tikhonov regularization problem. Therefore, a
 78 local minimizer of the original l_p problem can be found by a local minimizer of the l_2
 79 problem that is solved using the idea of Tikhonov EKI. As this transformation is ex-
 80 plicit and easy to calculate, the proposed method's overall computational complexity
 81 remains comparable to the complexity of Tikhonov EKI. In general, a transformed
 82 optimization problem can lead to additional difficulties, such as change of convexity,
 83 increased nonlinearity, additional/missing local minima of the original problem, etc.
 84 [14]. We show that the transformation does not add or remove local minimizers in
 85 the transformed formulation. A work imposing sparsity in EKI has been reported
 86 recently [31]. The idea of this work is to use thresholding and a l_1 constraint to
 87 impose sparsity in the inverse problem solution. The l_1 constraint is further relaxed

88 by splitting the solution into positive and negative parts. The split converts the l_1
 89 problem to a quadratic problem, while it still has a non-negativity constraint. On
 90 the other hand, our method does not require additional constraints by reformulating
 91 the optimization problem and works as a solver for the l_p regularized optimization
 92 problem (1.3).

93 This paper is structured as follows. Section 2 reviews the standard EKI and
 94 Tikhonov EKI. In section 3, we describe a transformation that converts the l_p reg-
 95 ularization problem (1.3), $0 < p \leq 1$, to the Tikhonov (that is, l_2) regularization
 96 problem, and provide the complete description of the l_p regularized EKI algorithm.
 97 We also discuss implementation and computation issues. Section 4 is devoted to the
 98 validation of the effectiveness and robustness of regularized EKI through a suite of
 99 numerical tests. The tests include a scalar toy problem with an analytic solution, a
 100 compressive sensing problem to benchmark with a convex l_1 minimization method,
 101 and a PDE-constrained nonlinear inverse problem from subsurface flow. We conclude
 102 this paper in section 5, discussing the proposed method's limitations and future work.

103 **2. Ensemble Kalman inversion.** The l_p regularized EKI uses a change of
 104 variables to transform a l_p problem into a l_2 problem, which is then solved by the
 105 standard EKI using an augmented measurement model. This section reviews the
 106 standard EKI and the application of the augmented measurement model in Tikhonov
 107 EKI to implement l_2 regularization. The review is intended to be concise, delivering
 108 the minimal ideas for the l_p regularized EKI. Detailed descriptions of the standard
 109 EKI and the Tikhonov EKI methods can be found in [20] and [9], respectively.

110 **2.1. Standard ensemble Kalman inversion.** EKI incorporates an artificial
 111 dynamics, which corresponds to the application of the forward model to each ensemble
 112 member. This application moves each ensemble member to the measurement space,
 113 which is then updated using the ensemble Kalman update formula. The ensemble
 114 updated by EKI stays in the linear span of the initial ensemble [20, 25]. Therefore, by
 115 choosing an initial ensemble appropriately for prior information, EKI is regularized
 116 as the ensemble is restricted to the linear span of the initial ensemble. Under a
 117 continuous-time limit, when the operator G is linear, it is proved in [30] that EKI
 118 estimate converges to the solution of the following optimization problem

$$119 \quad (2.1) \quad \underset{u \in \mathbb{R}^N}{\operatorname{argmin}} \frac{1}{2} \|y - G(u)\|_{\Gamma}^2.$$

120 In this paper, we consider the discrete-time EKI in [20], which is described below.

121 **Algorithm: standard EKI**

122 Assumption: an initial ensemble of size K , $\{u_0^{(k)}\}_{k=1}^K$ from prior information, is given.
 123 For $n = 1, 2, \dots$,

124 1. Prediction step using the artificial dynamics:

125 (a) Apply the forward model G to each ensemble member

$$126 \quad (2.2) \quad g_n^{(k)} := G(u_{n-1}^{(k)})$$

127 (b) From the set of the predictions $\{g_n^{(k)}\}_{k=1}^K$, calculate the mean and co-
 128 variances

$$129 \quad (2.3) \quad \bar{g}_n = \frac{1}{K} \sum_{k=1}^K g_n^{(k)},$$

130

$$\begin{aligned}
 (2.4) \quad C_n^{ug} &= \frac{1}{K} \sum_{k=1}^K (u_n^{(k)} - \bar{u}_n) \otimes (g_n^{(k)} - \bar{g}_n), \\
 C_n^{gg} &= \frac{1}{K} \sum_{k=1}^K (g_n^{(k)} - \bar{g}_n) \otimes (g_n^{(k)} - \bar{g}_n),
 \end{aligned}$$

132 where \bar{u}_n is the mean of $\{u_n^{(k)}\}$, i.e., $\frac{1}{K} \sum_{k=1}^K u_n^{(k)}$.

133 2. Analysis step:

134 (a) Update each ensemble member $u_n^{(k)}$ using the Kalman update

135 (2.5)
$$u_{n+1}^{(k)} = u_n^{(k)} + C_n^{ug} (C_n^{gg} + \Gamma)^{-1} (y_n^{(k)} - g_n^{(k)}),$$

136 where $y_{n+1}^{(k)} = y + \zeta_{n+1}^{(k)}$ is a perturbed measurement using Gaussian noise
137 $\zeta_{n+1}^{(k)}$ with mean zero and covariance Γ .

138 (b) Compute the mean of the ensemble as an estimate for the solution

139 (2.6)
$$\bar{u}_{n+1} = \frac{1}{K} \sum_{k=1}^K u_{n+1}^{(k)}$$

140 *Remark 2.1.* The term $C_n^{ug} (C_n^{gg} + \Gamma)^{-1}$ in (2.5) is from the Kalman gain matrix.
141 The standard EKI uses an extended space, $(u, G(u)) \in \mathbb{R}^{N+m}$, and then use the
142 Kalman update for the extended space variable. However, as we need to update only
143 u while $G(u)$ is subordinate to u , we have the update formula (2.5).

144 **2.2. Tikhonov ensemble Kalman inversion.** EKI is regularized through the
145 initial ensemble reflecting prior information. However, there are several numerical
146 evidence showing that EKI regularized only through an ensemble may have overfitting
147 [20]. Among other approaches to regularize EKI, Tikhonov EKI [9] uses the
148 idea of an augmented measurement to implement l_2 regularization, which is a simple
149 modification of the standard EKI. For the original measurement y , the augmented
150 measurement model extends y by adding the zero vector in \mathbb{R}^N , which yields an
151 augmented measurement vector $z \in \mathbb{R}^{m+N}$

152 (2.7) augmented measurement vector: $z = (y, 0)$.153 The forward model is also augmented to account for the augmented measurement
154 vector, which adds the identity measurement155 (2.8) augmented forward model: $F(u) = (G(u), u)$.156 Using the augmented measurement vector and the model, Tikhonov EKI has the
157 following inverse problem of estimating u from z 158 (2.9)
$$z = F(u) + \zeta.$$
159 Here ζ is a $m + N$ -dimensional measurement error for the augmented measurement
160 model, which is Gaussian with mean zero and covariance

161 (2.10)
$$\Sigma = \begin{pmatrix} \Gamma & 0 \\ 0 & \frac{1}{\lambda} I_N \end{pmatrix},$$

162 for the $N \times N$ identity matrix I_N .

163 The mechanism enabling the l_2 regularization in Tikhonov EKI is the incorporation
 164 of the l_2 penalty term as a part of the augmented measurement model. From the
 165 orthogonality between different components in \mathbb{R}^{m+N} , we have

$$166 \quad (2.11) \quad \begin{aligned} \frac{1}{2} \|z - F(u)\|_{\Sigma}^2 &= \frac{1}{2} \|y - G(u)\|_{\Gamma}^2 + \frac{1}{2} \|0 - u\|_{\frac{1}{\lambda} I_N}^2 \\ &= \frac{1}{2} \|y - G(u)\|_{\Gamma}^2 + \frac{\lambda}{2} \|u\|_2^2. \end{aligned}$$

167 Therefore, the standard EKI algorithm applied to the augmented measurement minimizes $\frac{1}{2} \|z - F(u)\|_{\Sigma}^2$, which equivalently minimizes the l_2 regularized problem.

169 **3. l_p -regularization for EKI.** This section describes a transformation that
 170 converts a l_p , $0 < p \leq 1$, regularization problem to a l_2 regularization problem. l_p -
 171 regularized EKI (l_p EKI), which we completely describe in [subsection 3.2](#), utilizes this
 172 transformation and solves the transformed l_2 regularization problem using the idea of
 173 Tikhonov EKI [9], the augmented measurement model.

174 **3.1. Transformation of l_p regularization into l_2 regularization.** For $0 <$
 175 $p \leq 1$, we define a function $\psi : \mathbb{R} \rightarrow \mathbb{R}$ given by

$$176 \quad (3.1) \quad \psi(x) = \text{sgn}(x)|x|^{\frac{p}{2}}, \quad x \in \mathbb{R}.$$

177 Here $\text{sgn}(x)$ is the sign function of x , which has 1 for $x > 0$, 0 for $x = 0$, and -1 for
 178 $x < 0$. It is straightforward to check that ψ is bijective and has an inverse $\xi : \mathbb{R} \rightarrow \mathbb{R}$
 179 defined as

$$180 \quad (3.2) \quad \xi(x) = \text{sgn}(x)|x|^{\frac{2}{p}}, \quad x \in \mathbb{R}.$$

181 For u in \mathbb{R}^N , we define a nonlinear map $\Psi : \mathbb{R}^N \rightarrow \mathbb{R}^N$, which applies ψ to each
 182 component of $u = (u_1, u_2, \dots, u_N)$,

$$183 \quad (3.3) \quad \Psi(u) = (\psi(u_1), \psi(u_2), \dots, \psi(u_N)).$$

184 As ψ has an inverse, the map Ψ also has an inverse, say Ξ

$$185 \quad (3.4) \quad \Xi(u) = \Psi^{-1}(u) = (\xi(u_1), \xi(u_2), \dots, \xi(u_N)).$$

186 For $v = \Psi(u)$, it can be checked that for each $i = 1, 2, \dots, N$,

$$187 \quad |v_i|^2 = |\psi(u_i)|^2 = |u_i|^p,$$

188 and thus we have the following norm relation

$$189 \quad (3.5) \quad \|v\|_2^2 = \|u\|_p^p.$$

190 This relation shows that the map $v = \Psi(u)$ converts the l_p -regularized optimization
 191 problem in u (1.3) to a l_2 regularized problem in v ,

$$192 \quad (3.6) \quad \underset{v \in \mathbb{R}^N}{\text{argmin}} \frac{\lambda}{2} \|v\|_2^2 + \frac{1}{2} \|y - \tilde{G}(v)\|_{\Gamma}^2,$$

193 where \tilde{G} is the pullback of G by Ξ

$$194 \quad (3.7) \quad \tilde{G} = G \circ \Xi.$$

195 A transformation between l_1 and l_2 regularization terms has already been used
 196 to solve an inverse problem in the Bayesian framework [32]. In the context of the
 197 randomize-then-optimize framework [2], the method in [32] draws a sample from a
 198 Gaussian distribution, which is then transformed to a Laplace distribution. As this
 199 method needs to match the corresponding densities of the variables (the original and
 200 the transformed variables) as random variables, the transformation involves calcula-
 201 tions related to cumulative distribution functions. For the scalar case, $v \in \mathbb{R}$, the
 202 transformation from l_2 to l_1 , denoted as gl , is given by

203 (3.8)
$$gl(v) = -\operatorname{sgn}(v) \log \left(1 - 2 \left| \phi(v) - \frac{1}{2} \right| \right).$$

204 where $\phi(u)$ is the cumulative distribution function of the standard Gaussian distribu-
 205 tion. Figure 1 shows the two transformations ξ (3.2) and gl (3.8); the former is based
 206 on the norm relation (3.5) and the latter is based on matching densities as random
 variables. We note that the transformation ξ has a region around 0 flatter than the

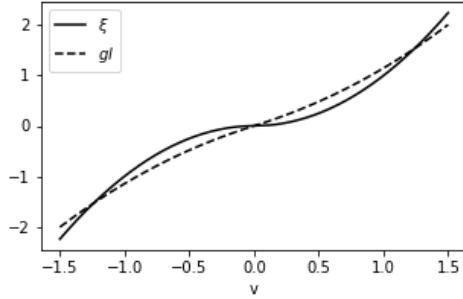


Fig. 1: ξ : transformation matching the norm relation (3.5), gl : transformation from Gaussian to Laplace distributions.

207
 208 transformation gl , but ξ diverts quickly as v moves further away from 0. From this
 209 comparison, we expect that the flattened region of ξ plays another role in imposing
 210 sparsity by trapping the ensemble to the flattened area.

211 In general, a reformulation of an optimization problem using a transformation has
 212 the following potential issues [14]: i) the degree of nonlinearity may be significantly
 213 increased, ii) the desired minimum may be inadvertently excluded, or iii) an additional
 214 local minimum can be included. In [10], for a non-convex problem, it is shown that
 215 TEKI converges to an approximate local minimum if the gradient and Hessian of the
 216 objective function are bounded. It is straightforward to check that the transformed
 217 objective function has bounded gradient and Hessian if $0 < p \leq 1$ regardless of
 218 the convexity of the problem. Therefore, if we can show that the original and the
 219 transformed problems have the same number of local minima, then it is guaranteed
 220 to find a local minimum of the original problem by finding a local minimum of the
 221 transformed problem using TEKI. We want to note the importance of the sign function
 222 in defining ψ and ξ . The sign function is not necessary to satisfy the norm relation
 223 (3.5), but it is essential to make the transformation Ψ and its inverse Ξ bijective.
 224 Without being bijective, the transformed l_2 problem can have more or less local
 225 minima than the original problem.

226 The following theorem shows that the transformation does not add or remove
 227 local minima.

228 **THEOREM 3.1.** *For an objective function $J(u) : \mathbb{R}^N \rightarrow \mathbb{R}$, if u^* is a local mini-
 229 mizer of $J(u)$, $\Psi(u^*)$ is also a local minimizer of $\tilde{J}(v) = J \circ \Xi(v)$. Similarly, if v^* is
 230 a local minimizer of $\tilde{J}(v)$, then $\Xi(v^*)$ is also a local minimizer of $J(u) = \tilde{J} \circ \Psi(u)$.*

231 *Proof.* From the definition (3.3) and (3.4), Ψ and Ξ are continuous and bijective.
 232 Thus for $u \in \mathbb{R}^N$, both Ψ and Ξ map a neighborhood of $u \in \mathbb{R}^N$ to neighborhoods of
 233 $\Psi(u)$ and $\Xi(u)$, respectively. As u^* is a local minimizer, there exists a neighborhood
 234 \mathcal{N} of u^* such that

235 (3.9)
$$J(u^*) \leq J(w) \quad \text{for all } w \in \mathcal{N}.$$

236 Let $v = \Psi(u^*)$ and $\mathcal{M} := \Psi(\mathcal{N})$ that is a neighborhood of v . For any $w \in \mathcal{M}$,
 237 $\Xi(w) \in \mathcal{N}$ and thus we have

238 (3.10)
$$\tilde{J}(v) = J(\Xi(v)) = J(u) \leq J(\Xi(w)) = \tilde{J}(w),$$

239 which shows that v is a local minimizer of \tilde{J} . The other direction is proved similarly
 240 by changing the roles of Ψ and Ξ and of J and \tilde{J} . \square

241 We note that an isolated local minimizer can replace the local minimizer in the
 242 theorem. If there is a unique global minimizer of the l_p regularization problem (1.3),
 243 the theorem guarantees that we can find it by finding the global minimizer of the l_2
 244 regularized problem (3.6).

245 **COROLLARY 3.2.** *For $0 < p \leq 1$, if the l_p regularized optimization (1.3) has
 246 a unique global minimizer, say u^\dagger , the l_2 regularized optimization (3.6) also has a
 247 unique global minimizer. By finding the minimizer u^\dagger of (3.6), say v^\dagger , u^\dagger is given by*

248 (3.11)
$$u^\dagger = \Xi(v^\dagger).$$

249 **3.2. Algorithm.** l_p -regularized EKI (l_p EKI) solves the transformed l_2 regular-
 250 ization problem using the standard EKI with the augmented measurement model. For
 251 the current study's completeness to implement l_p EKI, this subsection describes the
 252 complete l_p EKI algorithm and discuss issues related to implementation. Note that
 253 the Tikhonov EKI (TEKI) part in l_p EKI is slightly modified to reflect the setting
 254 assumed in this paper. The general TEKI algorithm and its variants can be found in
 255 [9].

256 We assume that the forward model G and the measurement error covariance Γ
 257 are known, and measurement $y \in \mathbb{R}^m$ is given (and thus $z = (y, 0)$ is also given).
 258 We also fix the regularization coefficient λ and p . Under this assumption, l_p EKI uses
 259 the following iterative procedure to update the ensemble until the ensemble mean

260
$$\bar{v} = \frac{1}{K} \sum_{k=1}^K v^{(k)}$$
 converges.

261 **Algorithm: l_p -regularized EKI**

262 Assumption: an initial ensemble of size K , $\{v_0^{(k)}\}_{k=1}^K$, is given.
 263 For $n = 1, 2, \dots$,

264 1. Prediction step using the forward model:
 265 (a) Apply the augmented forward model F to each ensemble member

266 (3.12)
$$f_n^{(k)} := F(v_n^{(k)}) = (\tilde{G}(v_n^{(k)}), v_n^{(k)})$$

267 (b) From the set of the predictions $\{f_n^{(k)}\}_{k=1}^K$, calculate the mean and co-
268 variances

269 (3.13)
$$\bar{f}_n = \frac{1}{K} \sum_{k=1}^K f_n^{(k)},$$

270 (3.14)
$$C_n^{vf} = \frac{1}{K} \sum_{k=1}^K (v_n^{(k)} - \bar{v}_n) \otimes (f_n^{(k)} - \bar{f}_n),$$

271
$$C_n^{ff} = \frac{1}{K} \sum_{k=1}^K (f_n^{(k)} - \bar{f}_n) \otimes (f_n^{(k)} - \bar{f}_n)$$

272 where \bar{v}_n is the ensemble mean of $\{v_n^{(k)}\}$, i.e., $\frac{1}{K} \sum_{k=1}^K v_n^{(k)}$.

273 2. Analysis step:

274 (a) Update each ensemble member $v_n^{(k)}$ using the Kalman update

275 (3.15)
$$v_{n+1}^{(k)} = v_n^{(k)} + C_n^{vf} (C_n^{ff} + \Sigma)^{-1} (z_{n+1}^{(k)} - f_n^{(k)}),$$

276 where $z_{n+1}^{(k)} = z + \zeta_{n+1}^{(k)}$ is a perturbed measurement using Gaussian noise
277 $\zeta_{n+1}^{(k)}$ with mean zero and covariance Σ .

278 (b) For the ensemble mean \bar{v}_n , the l_p EKI estimate, u_n , for the minimizer of
279 the l_p regularization is given by

280 (3.16)
$$u = \Xi(\bar{v}_n).$$

281 *Remark 3.3.* In EKI and TEKI, the covariance of $\zeta_{n+1}^{(k)}$ can be set to zero so that
282 all ensemble member uses the same measurement z without perturbations. In our
283 study, we focus on the perturbed measurement using the covariance matrix Γ .

284 *Remark 3.4.* The above algorithm is equivalent to TEKI, except that the forward
285 model G is replaced with the pullback of G by the transformation Ξ . In comparison
286 with TEKI, the additional computational cost for l_p EKI is to calculate the Transform-
287 ation $\Xi(v)$. In comparison with the standard EKI, the additional cost of l_p EKI, in
288 addition to the cost related to the transformation, is the matrix inversion $(C_n^{gg} + \Sigma)^{-1}$
289 in the augmented measurement space \mathbb{R}^{m+N} instead of a matrix inversion in the
290 original measurement space \mathbb{R}^m . As the covariance matrices are symmetric positive
291 definite, the matrix inversion can be done efficiently.

292 *Remark 3.5.* In l_p EKI, it is also possible to consider estimating u by transforming
293 each ensemble member and take average of the transformed members, that is,

294 (3.17)
$$u = \frac{1}{K} \sum_{k=1}^K \Xi(v_n^{(k)})$$

295 instead of (3.16). If the ensemble spread is large, these two approaches will make a
296 difference. In our numerical tests in the next section, we do not incorporate covari-
297 ance inflation. Thus the ensemble spread becomes relatively small when the estimate
298 converges, and thus (3.16) and (3.17) are not significantly different. In this study, we
299 use (3.16) to measure the performance of l_p EKI.

300 In recovering sparsity using the l_p penalty term, if the penalty term's convexity is
301 not necessary, it is preferred to use a small $p < 1$ as a smaller p imposes stronger spar-
302 sity. The optimization problem (1.3) can be interpreted as a constrained optimization
303 problem that minimizes the l_p term of u with a constraint related to the data. That
304 is, the solution to the optimization problem is an intersection point of an l_p ball and
305 an affine subspace [12]. For $p \leq 1$, the intersection point is expected to take place
306 on the axes and thus lead to a sparse solution. In particular, it can be checked that
307 a small $p < 1$ has a high chance to have the intersection point at the axes, which
308 can impose stronger sparsity than a larger p . The transformation in l_p EKI works
309 for any positive p , but the transformation can lead to an overflow for a small p ; the
310 function ξ depends on an exponent $\frac{2}{p}$ that becomes large for a small p . Therefore,
311 there is a limit for the smallest p . In our numerical experiments in the next section,
312 the smallest p is 0.7 in the compressive sensing test.

313 There is a variant of l_p EKI worth further consideration. In [30], a continuous-
314 time limit of EKI has been proposed, which rescales $\Gamma \rightarrow h^{-1}\Gamma$ using $h > 0$ so
315 that the matrix inversion $(C_n^{gg} + h^{-1}\Gamma)^{-1}$ is approximated by $h\Gamma^{-1}$ as a limit of
316 $h \rightarrow 0$. In many applications, the measurement error covariance is assumed to be
317 diagonal. That is, the measurement error corresponding to different components are
318 uncorrelated. Thus the inversion Γ^{-1} becomes a cheap calculation in the continuous-
319 time limit. The continuous-time limit is then discretized in time using an explicit time
320 integration method with a finite time step. The latter is called 'learning rate' in the
321 machine learning community, and it is known that an adaptive time-stepping to solve
322 an optimization often shows improved results [11, 28]. The current study focuses on
323 the discrete-time update described in (2.5) and we leave adaptive time-stepping for
324 future work.

325 **4. Numerical tests.** We apply l_p -regularized EKI (l_p EKI) to a suite of inverse
326 problems to check its performance in regularizing EKI and recovering sparse structures
327 of solutions. The tests include: i) a scalar toy model where an analytic solution is
328 available, ii) a compressive sensing problem to recover a sparse signal from random
329 measurements of the signal, iii) an inverse problem in subsurface flow; estimation of
330 permeability from measurements of hydraulic pressure field whose forward model is
331 described by a 2D elliptic partial differential equation [8, 27]. In all tests, we run
332 l_p EKI for various values of $p \leq 1$, and compare with the result of Tikhonov EKI. We
333 analyze the results to check how effectively l_p EKI implements l_p regularization and
334 recover sparse solutions. When available, we also compare l_p EKI with a l_1 convex
335 minimization method. As quantitative measures for the estimation performance, we
336 calculate the l_1 error of the l_p EKI estimates and the data misfit $\|y - G(u)\|_2$.

337 Several parameters are to be determined in l_p EKI to achieve robust estimation
338 results, regularization coefficient λ , regularization power p , ensemble size, and its
339 initialization. In this study, to focus on implementing l_p regularization for EKI with-
340 out the effect of any particular strategy to choose the regularization coefficient, we
341 find the coefficient by hand-tuning so that l_p EKI achieves the best result for a given
342 p . In particular, we test λ that corresponds to $a \times 10^b$ where $a \in \{1, 2, \dots, 9\}$ and
343 $b \in \{-2, -1, \dots, 3\}$ and select the result with the smallest l_1 error. We leave the
344 l_p EKI performance investigation using other methods to choose λ , for example, cross-
345 validation, as future work. In choosing the regularization power p , we also use a
346 hand-tuning process. We gradually decrease p from 1 until l_p EKI diverges. Once we
347 find the lower bound for p , we tune λ to obtain the best result for the lower bound p .
348

349 Ensemble initialization plays a role in regularizing EKI, restricting the estimate
 350 to the linear span of the initial ensemble. In our experiments, instead of tuning the
 351 initial ensemble for improved results, we initialize the ensemble using a Gaussian
 352 distribution with mean zero and a constant diagonal covariance matrix (the variance
 353 will be specified later for each test). As this initialization does not utilize any prior
 354 information, a sparse structure in the solution, we regularize the solution mainly
 355 through the l_p penalty term. For each test, we run 100 trials of l_p EKI through 100
 356 realizations of the initial ensemble distribution and use the estimate averaged over
 357 the trials along with its standard deviation to measure the performance difference.
 358 We note that we tune λ for one trial and use the same λ for the other trials.

359 Regarding the ensemble size, for the scalar toy and the compressive sensing prob-
 360 lems, we test ensemble sizes larger than the dimension of u , the unknown variable
 361 of interest. The purpose of a large ensemble size is to minimize the sampling er-
 362 ror while we focus on the regularization effect of l_p EKI. To show the applicability of
 363 l_p EKI for high-dimensional problems, we also test a small ensemble size using the idea
 364 of multiple batches used in [29]. The multiple batch approach runs several batches
 365 where small magnitude components are removed after each batch. After removing
 366 small magnitude components from the previous batch, the ensemble is used for the
 367 next batch. The multiple batch approach enables a small ensemble size, 50 ensemble
 368 members, for the compressive sensing and the 2D elliptic inversion problems where
 369 the dimensions of u are 200 and 400, respectively.

370 In ensemble-based Kalman filters, covariance inflation is an essential tool to sta-
 371 bilize and improve the performance of the filters. In a connection with the inflation,
 372 an adaptive time-stepping has been investigated to improve the performance of EKI.
 373 Although the adaptive time-stepping can be incorporated in l_p EKI for performance
 374 improvements, we use the discrete version l_p EKI described in subsection 3.2 focus-
 375 ing on the effect of different types of regularization on inversion. We will report a
 376 thorough investigation along the line of adaptive time-stepping in another place.

377 **4.1. A scalar toy problem.** The first numerical test is a scalar problem for
 378 $u \in \mathbb{R}$ with an analytic solution. As this is a scalar problem, there is no effect
 379 of regularization from ensemble initialization, and we can see the effect from the l_p
 380 penalty term. The scalar optimization problem we consider here is the minimization
 381 of an objective function $J(u) = \frac{1}{4}|u|^p + \frac{1}{2}(1-u)^2$

$$382 \quad (4.1) \quad \underset{u \in \mathbb{R}}{\operatorname{argmin}} J(u) = \underset{u \in \mathbb{R}}{\operatorname{argmin}} \frac{1}{4}|u|^p + \frac{1}{2}(1-u)^2.$$

383 This setup is equivalent to solving the optimization problem (1.3) using l_p regular-
 384 ization with $\lambda = 1/2$, where $y = 1$, $G(u) = u$, and η is Gaussian with mean zero and
 385 variance 1. Using the transformation $v = \Psi(u) = \psi(u) = \operatorname{sgn}(u)|u|^{\frac{p}{2}}$ defined in (3.1),
 386 l_p EKI minimizes a transformed objective function $\tilde{J}(v) = \frac{1}{4}|v|^2 + \frac{1}{2}(1 - \operatorname{sgn}(v)|v|^{2/p})^2$

$$387 \quad (4.2) \quad \underset{v \in \mathbb{R}}{\operatorname{argmin}} \tilde{J}(v) = \underset{v \in \mathbb{R}}{\operatorname{argmin}} \frac{1}{4}|v|^2 + \frac{1}{2}(1 - \operatorname{sgn}(v)|v|^{2/p})^2,$$

388 which is an l_2 regularization of $\frac{1}{2}(1 - \operatorname{sgn}(v)|v|^{\frac{2}{p}})^2$.

389 For $p = 1$, the first row of Figure 2 shows the objective functions of l_p (4.1) and
 390 the transformed l_2 (4.2) formulations. Each objective function has a unique global
 391 minimum without other local minima. The minimizers are $\frac{3}{4}$ and $\frac{\sqrt{3}}{2}$ for l_1 and
 392 l_2 , respectively. We can check that the transformation does not add/remove local

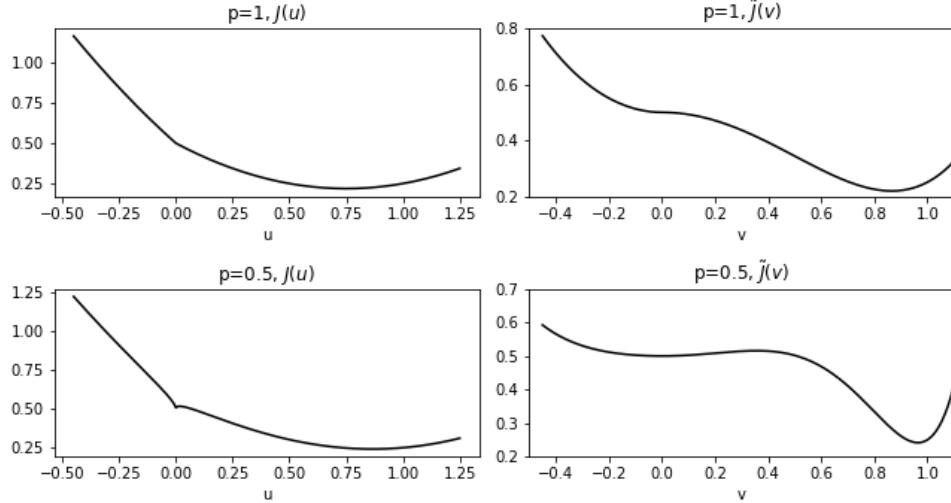


Fig. 2: Objective functions of (4.1) and (4.2) for $p = 1$ (first row) and $p = 0.5$ (second row).

393 minimizers, but the convexity of the objective function changes. The transformed
 394 objective function \tilde{J} has an inflection point at $u = 0$, which is also a stationary
 395 point. Note that the original function has no other stationary points than the global
 396 minimizer.

397 When $p = 0.5$, a potential issue of the transformation can be seen explicitly. The
 398 original objective and the transformed objective functions are shown in the second
 399 row of Figure 2. Due to the regularization term with $p = 0.5$, the objective functions
 400 are non-convex and have a local minimizer at $u = v = 0$ in addition to the global
 401 minimizers. In the transformed formulation (bottom right of Figure 2), the objective
 402 function flattens around $v = 0$, which shows a potential issue of trapping ensemble
 403 members around $v = 0$. Numerical experiments show that if the ensemble is initialized
 404 with a small variance, the ensemble is trapped around $v = 0$. On the other hand, if the
 405 ensemble is initialized with a sufficiently large variance (so that some of the ensemble
 406 members are initialized out of the well around $v = 0$), l_p EKI shows convergence to
 407 the true minimizer, $v = 0.9304$ (or $u = 0.8656$) even when it is initialized around 0.

408 We use 100 different realizations for the ensemble initialization and each trial
 409 uses 50 ensemble members. The estimates at each iteration, which is averaged over
 410 different trials, are shown in Figure 3. For $p = 1$ (first row) and $p = 0.5$ (second row),
 411 the left and right columns show the results when the ensemble is initialized with mean
 412 1 and 0, respectively. When $p = 1$ and initialized around 1, the ensemble estimate
 413 quickly converges to the true value 0.75 as the objective function is convex, and the
 414 initial guess is close to the true value. When $p = 0.5$, as the objective function is
 415 non-convex due to the regularization term, the convergence is slower than the $p = 1$
 416 case. When the ensemble is initialized around 0 for $p = 0.5$, a local minimizer, the
 417 ensemble needs to be initialized with a large variance. Using variance 1, which is 10
 418 times larger than 0.1, the variance for the ensemble initialization around 1, l_p EKI
 419 converges to the true value. The performance difference between different trials is

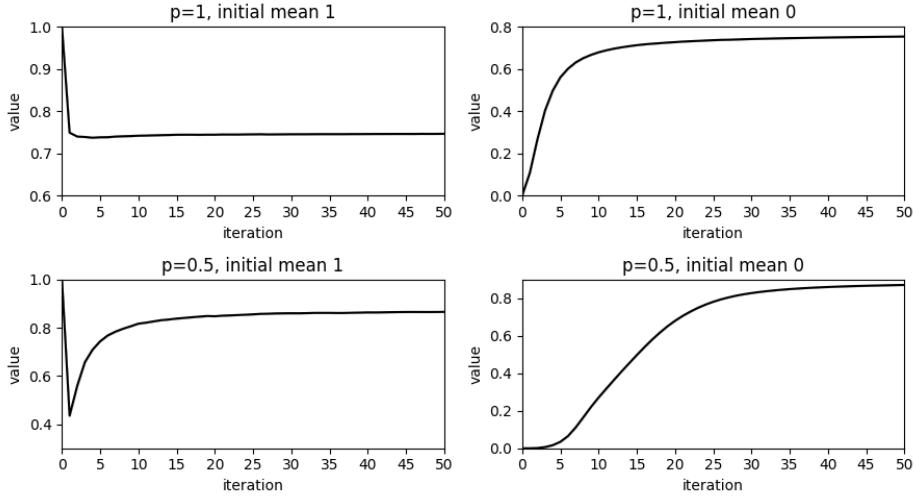


Fig. 3: Time series of l_p EKI estimate, $\xi(\bar{v}_n)$, which is averaged over 100 different trials.

420 marginal. The standard deviations of the estimate after 50 iterations are 6.62×10^{-3}
 421 ($p = 1$ initialized with 1), 7.95×10^{-3} ($p = 1$ initialized with 0), 8.79×10^{-3} ($p = 0.5$
 422 initialized with 1), and 1.14×10^{-2} ($p = 0.5$ initialized with 0). As a reference, the
 423 estimate using the transformation (3.8) based on matching the densities of random
 424 variables converges to 0.71.

425 **4.2. Compressive sensing.** The second test is a compressive sensing problem.
 426 The true signal u is a vector in \mathbb{R}^{200} , which is sparse with only four randomly selected
 427 non-zero components (their magnitudes are also randomly chosen from the standard
 428 normal distribution.) The forward model $G : \mathbb{R}^{200} \rightarrow \mathbb{R}^{20}$ is a random Gaussian
 429 matrix of size 20×200 , which yields a measurement vector in \mathbb{R}^{20} . The measurement
 430 y is obtained by applying the forward model to the true signal u polluted by Gaussian
 431 noise with mean zero and variance 0.01

432 (4.3)
$$y = Gu + \eta, \quad G \in \mathbb{R}^{20 \times 200}, \eta \sim \mathcal{N}(0, 0.01).$$

433 As the forward model is linear, several robust methods can solve the sparse recovery
 434 problem, including the l_1 convex minimization method [4]. This test aims to compare
 435 the performance of l_p EKI for various p values, rather than to advocate the use of
 436 l_p EKI over other standard methods. As the forward model is linear and cheap to
 437 calculate, the standard methods are preferred over l_p EKI for this test.

438 We first use a large ensemble size, 2000 ensemble members, to run l_p EKI. The
 439 ensemble is initialized by drawing samples from a Gaussian distribution with mean
 440 zero and a diagonal covariance (which yields variance 0.1 for each component). For
 441 $p = 1$ and 0.7, the tuned regularization coefficients, λ , are 100 and 300. When $p = 2$,
 442 which corresponds to TEKI, the best result can be obtained using λ ranging from
 443 10 to 200; we use the result of $\lambda = 50$ to compare with the other cases. For $p = 1$,
 444 we also compare the result of the convex l_1 minimization method using the interior
 445 point method using the Karush-Kuhn-Tucker condition [5] implemented in the Python
 446 library CVXOPT [26].

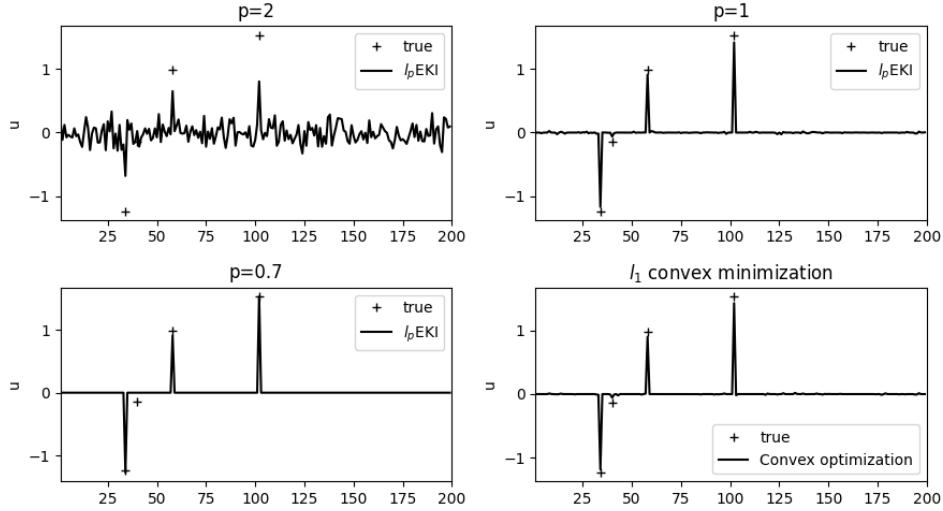


Fig. 4: Compressive sensing. Reconstruction of sparse signal using l_p EKI for $p=2$, 1 , and 0.7 . Ensemble size is 2000 . The bottom right plot is the reconstruction using the convex l_1 minimization method. For the true signal, only the nonzero components are marked.

447 Figure 4 shows the l_p EKI estimates after 20 iterations averaged over 100 trials
 448 for $p = 2$ (top left), $p = 1$ (top right), and $p = 0.7$ (bottom left), along with the
 449 estimate by the convex optimization (bottom right). As it is well known in compressive
 450 sensing, l_2 regularization fails to capture the true signal's sparse structure. As p
 451 decreases to 1 , l_p EKI develops sparsity in the estimate, comparable to the estimate
 452 of the convex l_1 minimization method. The slightly weak magnitudes of the three
 453 most significant components by l_p EKI improve as p decreases to 0.7 . When $p = 0.7$,
 454 l_p EKI captures the correct magnitudes at the cost of losing the smallest magnitude
 455 component. The smallest magnitude component can be captured if the regularization
 456 coefficient λ decreases to 20 (see the left plot of Figure 5 for the l_p EKI estimate with
 457 $\lambda = 20$). However, this estimate also has several artificial non-zero components, which
 458 increases the l_1 error by about 15%. We note that the smallest magnitude component
 459 is challenging to capture; the magnitude is comparable to the measurement error
 460 $0.1 = \sqrt{0.01}$. When the measurement error variance decreases by a factor of 10 ,
 461 l_p EKI with $p = 0.7$ captures the smallest magnitude component with less significant
 462 artificial non-zero components (the right plot of Figure 5).

463 Another cost of using $p < 1$ to impose stronger sparsity than $p = 1$ is a slow
 464 convergence rate of l_p EKI. The time series of the l_1 estimation error and the data
 465 misfit of l_p EKI averaged over 100 trials are shown in Figure 6 alongside those of the
 466 convex optimization method. The results show that $p = 0.7$ converges slower than
 467 $p = 1$ (see Table 1 for the numerical values of the error and the misfit). Although
 468 there is a slowdown in convergence, it is worth noting that l_p EKI with $p = 0.7$
 469 converges in a reasonably short time, 15 iterations, to achieve the best result. l_p EKI
 470 with $p = 2$ converges fast with the smallest data misfit. In this case, by combining
 471 many columns of G , l_p EKI makes a good approximation to the measurement error,

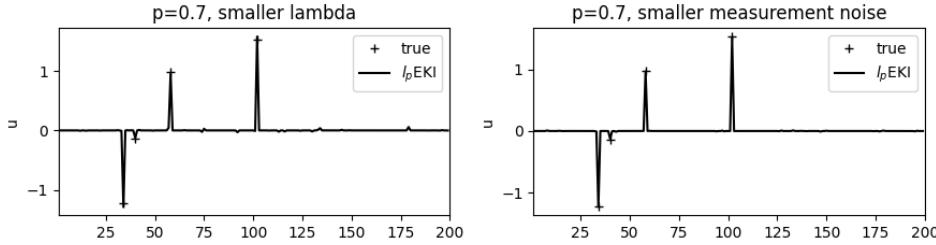


Fig. 5: l_p EKI estimates capturing the smallest magnitude component. Left: uses a smaller $\lambda = 20$. Right: uses a smaller measurement error variance 10^{-3} .

Method	l_1 error	data misfit
$p = 2$, ens size 2000	14.0802	0.0515
$p = 1$, ens size 2000	0.7848	0.8018
$p = 0.7$, ens size 2000	0.2773	1.2737
$p = 1$, ens size 50	1.6408	1.4095
$p = 0.7$, ens size 50	0.6027	1.8958
l_1 convex minimization	0.5623	0.9030

Table 1: Compressive sensing. l_p EKI estimate l_1 error and data misfit for $p = 2, 1$ and 0.7.

472 which yields a data misfit smaller than the actual norm of the measurement error
 473 0.6014. In comparison, the other methods have misfits larger than the measurement
 474 norm. However, the l_2 regularization is not strong enough to impose sparsity in the
 475 estimate and yields the largest estimation error, which is 20 times larger than the case
 476 of $p = 1$. Note that the convex optimization method has the fastest convergence rate;
 477 it converges within three iterations and captures the four nonzero components with
 478 slightly smaller magnitudes than $p = 0.7$ for the three most significant components.

479 The ensemble size 2000 is larger than the dimension of the unknown vector u ,
 480 200. A large ensemble size can be impractical for a high-dimensional unknown vector.
 481 To see the applicability of l_p EKI using a small ensemble size, we use 50 ensemble
 482 members and two batches following the multiple batch approach [29]. The first batch
 483 runs 10 iterations, and all components whose magnitudes are less than 0.1 (the square
 484 root of the observation variance) are removed. The problem's size the second batch
 485 solves ranges from 30-45 (depending on a realization of the initial ensemble), which
 486 is then solved for another 10 iterations. The estimates using 50 ensemble members
 487 for $p = 1$ and $p = 0.7$ after two batch runs (i.e., 20 iterations) are shown in Figure 7.
 488 Compared with the large ensemble size case, the small ensemble size run also captures
 489 the most significant components at the cost of fluctuating components larger than the
 490 large ensemble size test. We note that the estimates are averaged over 100 trials, and
 491 thus there are components whose magnitudes are less than the threshold value 0.1
 492 used in the multiple batch run.

493 As a measure to check the performance difference for different trials, Figure 8
 494 shows the standard deviations of l_p EKI estimates for $p = 1$ and 0.7 after 20 iterations.
 495 The first row shows the results using 2000 ensemble members, while the second row

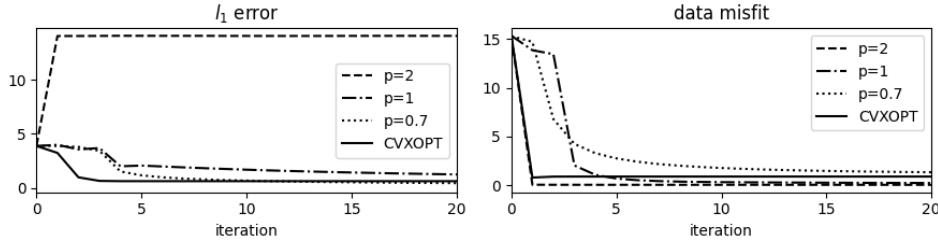


Fig. 6: Compressive sensing. l_1 error of the l_p EKI estimate and data misfit.

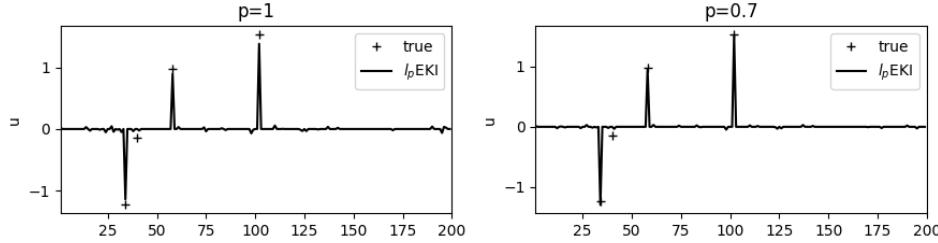


Fig. 7: Compressive sensing. Reconstruction of sparse signal using l_p EKI for $p=1$ and 0.7 . Ensemble size is 50. For the true signal, only the nonzero components are marked.

496 shows the ones using 50 ensemble members. The standard deviations of the large
 497 ensemble size are smaller than those of the small ensemble size case as the large
 498 ensemble size has a smaller sampling error. In all cases, the standard deviations are
 499 smaller than 6% of the magnitude of the most significant components. In terms of p ,
 500 the standard deviations of $p = 0.7$ are smaller than those of $p = 1$.

501 **4.3. 2D elliptic problem.** Next, we consider an inverse problem where the
 502 forward model is given by an elliptic partial differential equation. The model is
 503 related to subsurface flow described by Darcy flow in the two-dimensional unit square
 504 $(0, 1)^2 \subset \mathbb{R}^2$

505 (4.4)
$$-\nabla \cdot (k(x)\nabla p(x)) = f(x), \quad x = (x_1, x_2) \in (0, 1)^2.$$

506 The scalar field $k(x) > \alpha > 0$ is the permeability, and another field $p(x)$ is the
 507 piezometric head or the pressure field of the flow. For a known source term $f(x)$, the
 508 inverse problem estimates the permeability from measurements of the pressure field
 509 p . This model is a standard model for an inverse problem in oil reservoir simulations
 510 and has been actively used to measure EKI's performance and its variants, including
 511 TEKI [20, 9].

512 We follow the same setting used in TEKI [9] for the boundary conditions and the
 513 source term. The boundary conditions consist of Dirichlet and Neumann boundary
 514 conditions

515
$$p(x_1, 0) = 100, \frac{\partial p}{\partial x_1}(1, x_2) = 0, -k \frac{\partial p}{\partial x_1}(0, x_2) = 500, \frac{\partial p}{\partial x_2}(x_1, 1) = 0,$$

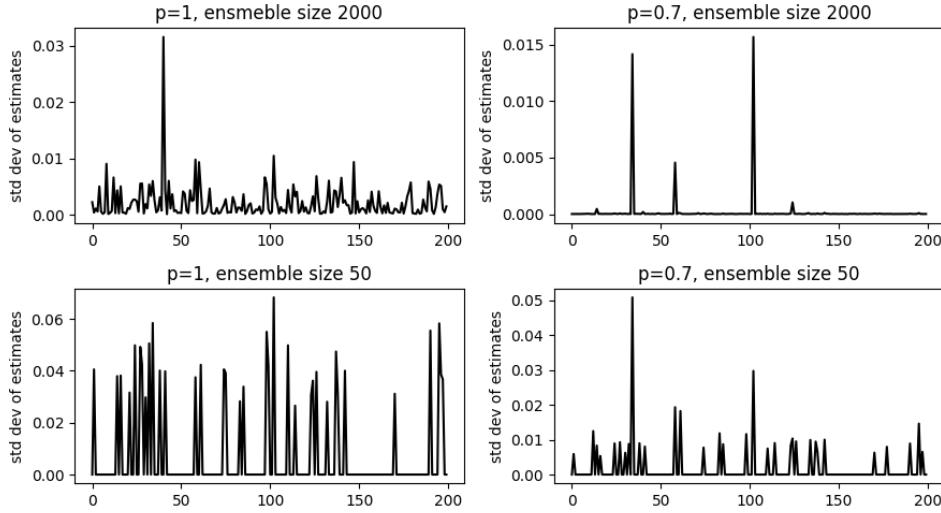


Fig. 8: Compressive sensing. Standard deviation of the estimates using 100 trials.

516 and the source term is piecewise constant

$$517 \quad f(x_1, x_2) = \begin{cases} 0 & \text{if } 0 \leq x_2 \leq \frac{4}{6}, \\ 137 & \text{if } \frac{4}{6} < x_2 \leq \frac{5}{6}, \\ 274 & \text{if } \frac{5}{6} < x_2 \leq 1. \end{cases}$$

518 A physical motivation of the above configuration can be found in [8]. We use 15×15
 519 regularly spaced points in $(0, 1)^2$ to measure the pressure field with a small measure-
 520 ment error variance 10^{-6} . For a given k , the forward model is solved by a FEM
 521 method using the second-order polynomial basis on a 60×60 uniform mesh.

522 In addition to the standard setup, we impose a sparse structure in the permeabil-
 523 ity. We assume that the log permeability, $\log k$, can be represented by 400 components
 524 in the cosine basis $\phi_{ij} = \cos(i\pi x_1) \cos(j\pi x_2)$, $i, j = 0, 1, \dots, 19$,

$$525 \quad (4.5) \quad \log k(x) = \sum_{i,j=0}^{19} u_{ij} \phi_{ij}(x),$$

526 where only six of $\{u_{ij}\}$ are nonzero. That is, we assume that the discrete cosine
 527 transform of $\log k$ is sparse with only 6 nonzero components out of 400 components.
 528 Thus, the problem we consider here can be formulated as an inverse problem to re-
 529 cover $u = \{u_{ij}\} \in \mathbb{R}^{400}$ (which has only six nonzero components) from a measurement
 530 $y \in \mathbb{R}^{225}$, the measurement of p at 15×15 regularly spaced points. In terms of spar-
 531 sity reconstruction, the current setup is similar to the previous compressive sensing
 532 problem, but the main difference lies in the forward model. In this test, the forward
 533 model is nonlinear and computationally expensive to solve, where the forward model
 534 in the compressive sensing test was linear using a random measurement matrix.

535 For this test, we run l_p EKI using only a small ensemble size due to the high
 536 computational cost of running the forward model. As in the previous test, we use the
 537 multiple batch approach. First, the l_p EKI ensemble of size 50 is initialized around

p	l_1 error	data misfit
2	21.3389	4.1227
1	0.1553	0.5707
0.8	0.0719	0.5682

Table 2: 2D elliptic problem. l_p EKI estimate l_1 error and data misfit for $p = 2, 1$ and 0.8 .

538 zero with Gaussian perturbations of variance 0.1. After the first five iterations, all
 539 components whose magnitudes less than 5×10^{-3} are removed at each iteration. The
 540 threshold value is slightly smaller than the smallest magnitude component of the true
 541 signal. Over 100 different trials, the average number of nonzero components after 30
 542 iterations is 18 that is smaller than the ensemble size.

543 The true value of u used in this test and its corresponding log permeability, $\log k$,
 544 are shown in the first row of Figure 9 (u is represented as a one-dimensional vector
 545 by concatenating the row vectors of $\{u_{ij}\}$). The l_p EKI estimates for $p = 2, 1$, and 0.8
 546 are shown in the second to the fourth rows of Figure 9. Here $p = 0.8$ was the smallest
 547 value we can use for l_p EKI due to the numerical overflow in the exponentiation of
 548 $\log k$. A smaller p can be used with a smaller variance for ensemble initialization, but
 549 the gain is marginal. The results of l_p EKI are similar to the compressive sensing case.
 550 $p = 0.8$ has the best performance recovering the four most significant components of
 551 u . $p = 1$ has slightly weak magnitudes missing the correct magnitudes of the two most
 552 significant components (corresponding to one-dimensional indices 141 and 364). Both
 553 cases converge within 20 iterations to yield the best result (see Figure 10 and Table 2
 554 for the time series and numerical values of the l_1 error and data misfit). When $p = 2$,
 555 l_p EKI performs the worst; it has the largest l_1 error and data misfit. We note that
 556 $p = 2$ uses the result after running 50 iterations at which the estimate converges.

557 The performance difference between different trials is not significant. The stan-
 558 dard deviations of the l_p EKI estimates using 100 trials are shown in Figure 11. The
 559 standard deviations for nonzero components are larger than the other components,
 560 but the largest standard deviation is less than 3% of the magnitude of the true signal.
 561 As in the compressive sensing test, the deviations are slightly smaller for $p < 1$ than
 562 $p = 1$.

563 **5. Discussions and conclusions.** We have proposed a strategy to implement
 564 $l_p, 0 < p \leq 1$, regularization in ensemble Kalman inversion (EKI) to recover sparse
 565 structures in the solution of an inverse problem. The l_p -regularized ensemble Kalman
 566 inversion (l_p EKI) proposed here uses a transformation to convert the l_p regularization
 567 problem to the l_2 regularization problem, which is then solved by the standard EKI
 568 with an augmented measurement model used in Tikhonov EKI. We showed a one-
 569 to-one correspondence between the local minima of the original and the transformed
 570 formulations. Thus a local minimum of the original problem can be obtained by
 571 finding a local minimum of the transformed problem. As other iterative methods for
 572 non-convex problems, initialization plays a vital role in the proposed method's per-
 573 formance. The effectiveness and robustness of regularized EKI are validated through
 574 a suite of numerical tests, showing robust results in recovering sparse solutions using
 575 $p \leq 1$.

576 In implementing l_p regularization for EKI, there is a limit on $p < 1$ due to an
 577 overflow. One definitive source of the overflow is the transformation ξ that involves

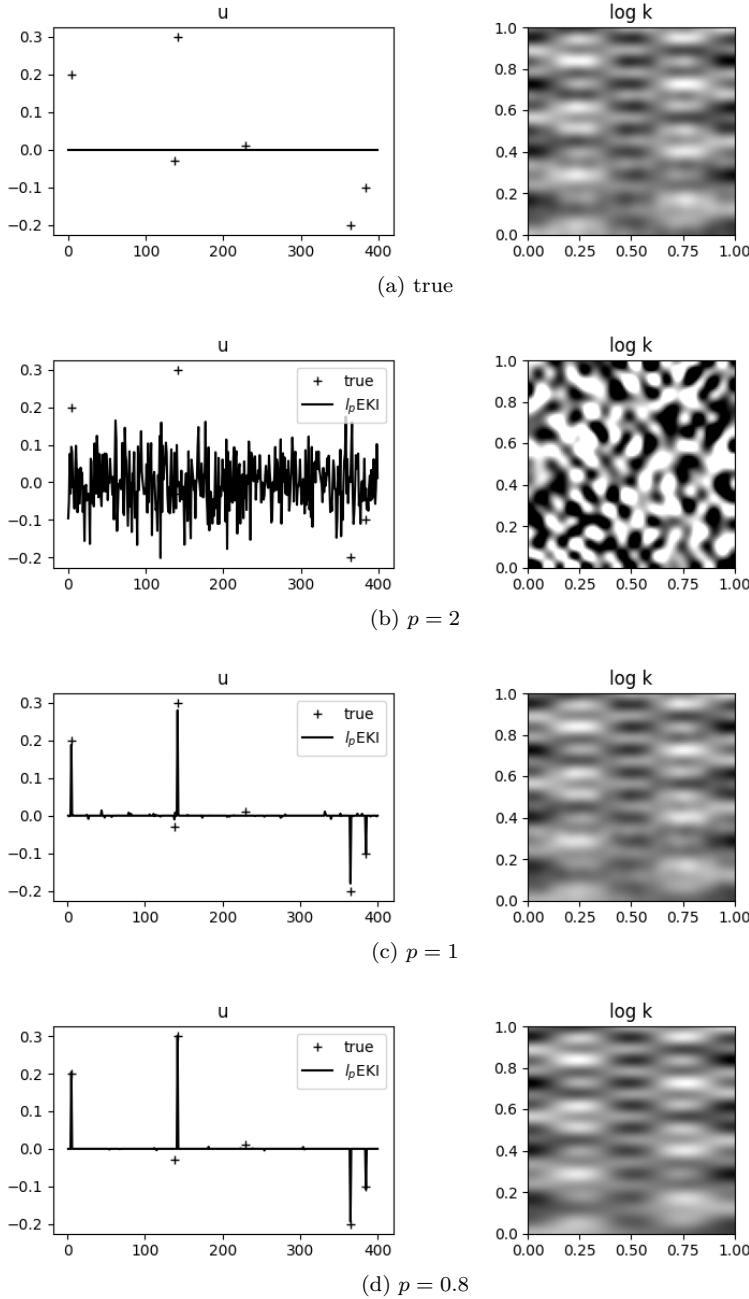


Fig. 9: 2D elliptic problem. Left column: the true u and l_p EKI estimates for $p = 2, 1$, and 0.8 . Right column: $\log k$ of the true and l_p EKI estimates. All plots have the same grey scale. $p = 1$ and 0.8 use the results after 20 iterations while $p = 2$ uses the result after 50 iterations. For the true signal, only the nonzero components are marked.

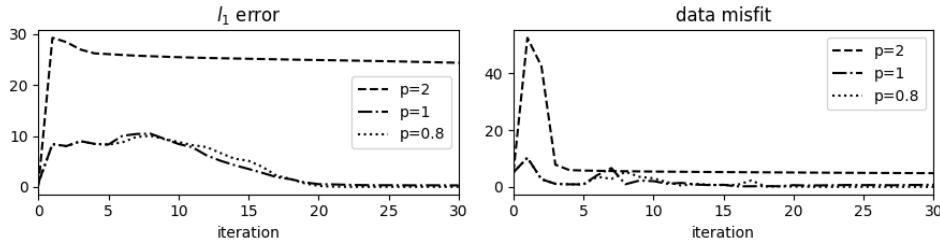


Fig. 10: 2D elliptic problem. l_1 error of the l_p EKI estimates and data misfit.

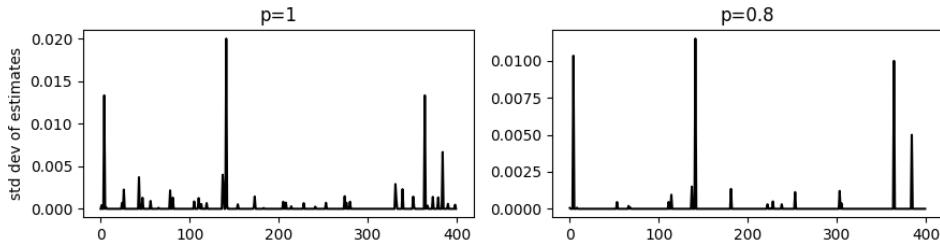


Fig. 11: 2D elliptic problem. Standard deviation of the estimates using 100 trials.

578 $\frac{2}{p}$ as an exponent. For a small $p < 1$, the transformation ξ can diverge, and thus EKI
 579 suffers from instability. One possible workaround is to impose the l_p penalty term
 580 directly in the fidelity term instead of transforming it to the l_2 regularization using ξ .
 581 The penalty term incorporated in the fidelity term can be achieved by an extended
 582 measurement framework similar to Tikhonov EKI but with a nonlinear measurement
 583 operator. Also, in the ensemble filters, the filter estimate can diverge to machine
 584 infinity under a stringent filter setup, which is called ‘catastrophic filter divergence’
 585 [19, 17]. It is shown in [22] that one of the mechanisms for the filter instability is
 586 related to the measurement operator. As l_p regularization in EKI is implemented
 587 through an extended measurement operator, it is natural to investigate a connection
 588 between the catastrophic filter divergence and the instability in l_p EKI for $p < 1$. In
 589 particular, it is worth considering several methods that prevent the catastrophic filter
 590 divergence, including adaptive inflation [33, 24], for stabilizing l_p EKI. The effect of
 591 the above-mentioned approaches in stabilizing l_p EKI for $p < 1$ is under investigation
 592 and will be reported in another place.

593 For successful applications of l_p EKI for high-dimensional inverse problems, it
 594 is essential to maintain a small ensemble size for efficiency. In the current study,
 595 we considered the multiple batch approach. The approach removes non-significant
 596 components after each batch, and thus the problem size (i.e., the dimension of the
 597 unknown signal) decreases over different batch runs. This approach enabled l_p EKI
 598 to use only 50 ensemble members to solve 200 and 400-dimensional inverse problems.
 599 Other techniques, such as variance inflation and localization, improve the performance
 600 of the standard EKI using a small ensemble size [30]. It would be natural to investigate
 601 if these techniques can be extended to l_p EKI to decrease the sampling error of l_p EKI.

602 In the current study, we have left several variants of l_p EKI for future work.

603 Weighted l_1 has been shown to recover sparse solutions using fewer measurements
 604 than the standard l_1 [7]. It is straightforward to implement weighted l_1 (and fur-
 605 ther weighted l_p for $p < 1$) in l_p EKI by replacing the identity matrix in (2.10) with
 606 another type of covariance matrix corresponding to the desired weights. We plan to
 607 study several weighting strategies to improve the performance of l_p EKI. As another
 608 variant of l_p EKI, we plan to investigate the adaptive time-stepping under the contin-
 609 uous limit. The time step for solving the continuous limit equation, which is called
 610 ‘learning rate’ in the machine learning community, is known to affect an optimization
 611 solver [11]. The standard ensemble Kaman inversion has been applied to machine
 612 learning tasks, such as discovering the vector fields defining a differential equation,
 613 using time series data [23] and sparse learning using thresholding [31]. We plan to
 614 investigate the effect of an adaptive time-stepping for performance improvements and
 615 compare with the sparsity EKI method using thresholding in dimension reduction in
 616 machine learning.

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