# Efficient Robust Parameter Identification in Generalized Kalman Smoothing Models 

Jonathan Jonker* Peng Zheng ${ }^{\dagger}$ Aleksandr Y. Aravkin ${ }^{\dagger}$


#### Abstract

Dynamic inference problems in autoregressive (AR/ARMA/ARIMA), exponential smoothing, and navigation are often formulated and solved using state-space models (SSM), which allow a range of statistical distributions to inform innovations and errors. In many applications the main goal is to identify not only the hidden state, but also additional unknown model parameters (e.g. AR coefficients or unknown dynamics).

We show how to efficiently optimize over model parameters in SSM that use smooth process and measurement losses. Our approach is to project out state variables, obtaining a value function that only depends on the parameters of interest, and derive analytical formulas for first and second derivatives that can be used by many types of optimization methods.

The approach can be used with smooth robust penalties such as Hybrid and the Student's $\mathbf{t}$, in addition to classic least squares. We use the approach to estimate robust AR models and long-run unemployment rates with sudden changes.


## I. Introduction.

The linear state space model is widely used in tracking and navigation [4], control [1], signal processing [2], and other time series [6], [9]. The model assumes linear relationships between latent states with noisy observations:

$$
\begin{array}{ll}
x_{k}=G_{k} x_{k-1}+\epsilon_{k}^{p}, & k=1, \ldots, N, \\
z_{k}=H_{k} x_{k}+\epsilon_{k}^{m}, & k=1, \ldots, N \tag{1}
\end{array}
$$

where $x_{0}$ is a given initial state estimate, $x_{1}, \ldots, x_{N}$ are unknown latent states with known linear process models $G_{k}$, and $z_{1}, \ldots, z_{N}$ are observations obtained using known linear models $H_{k}$. The errors $\epsilon_{k}^{p}$ and $\epsilon_{k}^{m}$ are assumed to be mutually independent random variables with covariances $Q_{k}$ and $R_{k}$. These covariances may be singular to capture standard autoregressive structures.

In many applications the models $G_{k}, H_{k}, Q_{k}, R_{k}$ are specified up to model parameters $\theta$. We restrict out attention to formulations where variances $Q_{k}, R_{k}$ are known, while $G_{k}(\theta)$ and $H_{k}(\theta)$ are $\mathcal{C}^{2}$ mappings of $\theta$. This captures smoothing parameters in Holt-Winters c.f. [6], autoregressive and moving average parameters in ARMA c.f. [9], and unknown dynamic parameters in navigation models. In most of these models, $G$ and $H$ are affine functions of unknown parameters $\theta$.

Standard models assume the errors $\epsilon_{k}^{p}$ and $\epsilon_{k}^{m}$ are Gaussian, which gives rise to the least squares penalty in the inference problem, see the red solid curve in Figure 1 Changing the

[^0]

Fig. 1: Common smooth loss functions: least-squares (red solid), Hybrid (blue dashed), and student's T (violet dash dot).
observation model to the Hybrid (blue dash) or Student's $t$ loss (violet dash dot) robustifies model estimates in the face of measurement outliers. Analogous changes to the innovations model allows the framework to track sudden changes.

Motivating Application: Structural Unemployment Rate. We are interested in fitting parameters within structural unemployment rate models, see e.g. [8]. The state vector

$$
x_{k}=\left[\begin{array}{llll}
u_{k-1} & u_{k-1}^{c} & u_{k} & u_{k}^{c} \tag{2}
\end{array}\right]^{T}
$$

tracks total ( $u$ ) and 'cyclic' $\left(u^{c}\right)$ unemployment using the autoregressive model

$$
\begin{gather*}
G_{k}=\left[\begin{array}{cccc}
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
-l_{1} & 0 & 1+l_{1} & 0 \\
0 & 1 / 2-l_{2} & 0 & l_{2}
\end{array}\right], \quad \epsilon_{k}^{p}=\left[\begin{array}{c}
0 \\
0 \\
\epsilon_{k}^{1} \\
\epsilon_{k}^{2}
\end{array}\right]  \tag{3}\\
H_{k}=\left[\begin{array}{cccc}
0 & 0 & 1 & 1 \\
0 & \gamma / 2 & 0 & \gamma / 2
\end{array}\right], \quad \epsilon_{k}^{m}=\left[\begin{array}{c}
\epsilon_{k}^{3} \\
\epsilon_{k}^{4}
\end{array}\right] \tag{4}
\end{gather*}
$$

Here, $\ell_{1}$ and $\ell_{2}$ are auto-regressive parameters while $\gamma$ is an unknown measurement parameter. Unemployment rates can experience fast changes, so we need a heavy tailed model for innovations. To solve the full problem, we must

1) Estimate states $\left\{x_{k}\right\}$ as well as parameters $\ell_{1}, \ell_{2}, \gamma$.
2) Account for the singular process covariance $Q$.
3) Use non-Gaussian losses (e.g. Hybrid and Student's t) for $\epsilon_{k}^{p}$ to track fast rate changes.
The paper proceeds as follows. In Section III, we review optimization formulations for state and model parameter inference using singular and nonsingular covariance models, and introduce the value function which depends only on the model parameters, as e.g. $\ell_{1}, \ell_{2}, \gamma$ above. In Sections IV and $V$, we look in detail at nonsingular and singular Kalman smoothing
models, and obtain existence results and formulas for first and second derivatives of the value function. Finally, in Section VI we present use cases that show how to efficiently obtain structural parameters when using general losses and singular covariance structure.

## II. Notations and Preliminaries

We first introduce notation and key definitions.
a) Superscript and subscript: We use superscripts to distinguish process $(p)$ and measurement ( $m$ ) model variables and subscripts to represent partial derivatives $(\theta, y, r, \ldots)$ and the index in the Kalman model $(k)$. When taking derivatives, subscripts indicate the position rather than actual variable. For example, if we denote $v(\theta)=f(\theta, Y(\theta))$, then

$$
\nabla v(\theta) \neq f_{\theta}(\theta, Y(\theta))=\left.\partial_{\theta} f(\theta, y)\right|_{y=Y(\theta)}
$$

b) Loss functions: We use the following loss functions:

- Least squares: $\ell(r)=\frac{1}{2}\|r\|^{2}$.
- Hybrid: $\ell(r ; \nu)=\sum_{i} \sqrt{r_{i}^{2}+\nu^{2}}-\nu$.
- Student's T: $\ell(r ; \nu)=\sum_{i} \ln \left(1+r_{i}^{2} / \nu\right)$.


## III. Differentiating Implicit Functions

In this section, we introduce a general theoretical result for calculating the derivatives for implicit functions in an optimization context. We then specialize this general theorem to nonsingular and singular state space models (SSM) in the next section.

Consider a $\mathcal{C}^{2}$-smooth function, $f: \mathbb{R}^{n} \times \mathbb{R}^{m} \rightarrow \mathbb{R}$, where in SSM models we denote parameters by $\theta$ in $f(\theta, y)$ and the states together with any auxiliary variables (such as dual variables) by $y$. The appropriate stationary condition is given by

$$
\begin{equation*}
\mathcal{H}(\theta, y):=f_{y}(\theta, y)=0 \tag{5}
\end{equation*}
$$

For any given $\theta$, the optimal estimate $y(\theta)$ is obtained by solving the equation $\mathcal{H}(\theta, y)=0$; in particular $y(\theta)$ depends on $\theta$ implicitly. We introduce a variant of the implicit function theorem presented by [5] to characterize the structure of this implicit dependence.
Theorem 1 (Implicit Functions and Derivatives). Suppose that $\mathscr{U} \subset \mathbb{R}^{n}$ and $\mathscr{V} \subset \mathbb{R}^{m}$ are open, $\mathcal{H}: \mathscr{U} \times \mathscr{V} \rightarrow \mathbb{R}^{m}$ is continuously differentiable. If there exists $\bar{\theta} \in \mathscr{U}$ and $\bar{y} \in$ $\mathscr{V}$, such that $\mathcal{H}(\bar{\theta}, \bar{y})=0$ and $\mathcal{H}_{y}(\bar{\theta}, \bar{y})$ is invertible. Then there exists (if necessary we choose $\mathscr{U}$ and $\mathscr{V}$ to be small neighborhood of $\bar{\theta}$ and $\bar{y}$ to guarantee the existence) a $\mathcal{C}^{1}$ mapping $Y: \mathscr{U} \rightarrow \mathscr{V}$ satisfying $Y(\bar{\theta})=\bar{y}$, and $\mathcal{H}(\theta, Y(\theta))=$ 0 for all $\theta$ in $\mathscr{V}$.

Moreover, we have the formula

$$
Y_{\theta}(\theta)=-\mathcal{H}_{y}(\theta, Y(\theta))^{-1} \mathcal{H}_{\theta}(\theta, Y(\theta))
$$

When the function $Y(\theta)$ as above exists, we can define the value function

$$
\begin{equation*}
v(\theta)=f(\theta, Y(\theta)) \tag{6}
\end{equation*}
$$

Our goal is to compute first and second derivatives of $v$, which are summarized in the following corollary.

Corollary 1 (Derivatives of the Value Function (6)). Under the assumptions of Theorem 1] and using $\bar{y}$ to represent the $y$ obtained by evaluating $Y(\bar{\theta})$, we have,

$$
\begin{align*}
v_{\theta}(\bar{\theta}) & =f_{\theta}(\bar{\theta}, \bar{y}) \\
v_{\theta \theta}(\bar{\theta}) & =f_{\theta \theta}(\bar{\theta}, \bar{y})-\mathcal{H}_{\theta}(\bar{\theta}, \bar{y})^{\top} \mathcal{H}_{y}(\bar{\theta}, \bar{y})^{-1} \mathcal{H}_{\theta}(\bar{\theta}, \bar{y}) \tag{7}
\end{align*}
$$

These derivations are along the lines of those presented by Bell and Burke [5] and are mainly given here for a selfcontained exposition.

We now compute analytic expressions of derivatives with respect to model parameters for both nonsingular and singular Kalman smoothing systems.

## IV. Nonsingular SSM

Consider the case where the covariance matrices $Q_{k}$ and $R_{k}$ in SSM are nonsingular. Pre-whitening $\epsilon_{k}^{p}$ and $\epsilon_{k}^{m}$, the objective function of interest is given by

$$
\begin{align*}
f(\theta, y)= & \sum_{k=1}^{N}\left\{\ell_{k}^{p}\left(Q_{k}^{-1 / 2}\left(x_{k}-G_{k}(\theta) x_{k-1}\right)\right)\right.  \tag{8}\\
& \left.+\ell_{k}^{m}\left(R_{k}^{-1 / 2}\left(z_{k}-H_{k}(\theta) x_{k}\right)\right)\right\}
\end{align*}
$$

where $y=x=\left[x_{1} ; \ldots ; x_{N}\right], \ell_{k}^{p}$ and $\ell_{k}^{m}$ are the loss function corresponding to the distributions of $\epsilon_{k}^{p}$ and $\epsilon_{k}^{m}$. Here we assume $\ell_{k}^{p}, \ell_{k}^{m}$ are smooth; three key examples are least squares, Hybrid, and Student's $t$ losses introduced in Section II Objective (8) can be written compactly as,

$$
\begin{align*}
f(\theta, y)= & \ell^{p}\left(Q^{-1 / 2}(G(\theta) x-\zeta)\right)+  \tag{9}\\
& \ell^{m}\left(R^{-1 / 2}(H(\theta) x-z)\right)
\end{align*}
$$

where,
$G(\theta)=\left[\begin{array}{cccc}I & 0 & & \\ -G_{2}(\theta) & I & \ddots & \\ & \ddots & \ddots & 0 \\ & & -G_{N}(\theta) & I\end{array}\right], \quad Q=\left[\begin{array}{lll}Q_{1} & & \\ & \ddots & \\ & & Q_{N}\end{array}\right]$,
$H(\theta)=\left[\begin{array}{cccc}H_{1}(\theta) & 0 & \\ 0 & H_{2}(\theta) & \ddots & \\ & \ddots & \ddots & 0 \\ & & 0 & H_{N}(\theta)\end{array}\right], \quad R=\left[\begin{array}{lll}R_{1} & & \\ & \ddots & \\ & & R_{N}\end{array}\right]$,
and $\zeta=\left[x_{0} ; 0 ; \ldots ; 0\right]$ and $z=\left[z_{1} ; \ldots ; z_{N}\right]$.
The stationary condition in this case is given by

$$
\begin{align*}
\mathcal{H}(\theta, y) & =f_{y}(\theta, y) \\
& =G(\theta)^{\top} Q^{-\top / 2} \ell_{r}^{p}\left(r^{p}\right)+H(\theta)^{\top} R^{-\top / 2} \ell_{r}^{m}\left(r^{m}\right) \tag{10}
\end{align*}
$$

where $r^{p}=Q^{-1 / 2}(G(\theta) y-\zeta)$ and $r^{m}=R^{-1 / 2}(H(\theta) y-z)$.
In the least squares case, 10 is a linear equation solved by inverting the block-tridiagonal system

$$
G(\theta)^{\top} Q^{-1} G(\theta)+H(\theta)^{\top} R^{-1} H(\theta)
$$

for more general smooth penalties $\ell^{p}, \ell^{m}$ a Newton method is needed to compute $y(\theta)$.

By Theorem 1, existence and differentiability of $Y(\theta)$ is guaranteed by the existence of the pair $(\bar{\theta}, \bar{y})$ such that, $\mathcal{H}(\bar{\theta}, \bar{y})=0$ and the partial Hessian below is invertible:

$$
\begin{aligned}
\mathcal{H}_{y}(\bar{\theta}, \bar{y})= & G(\bar{\theta})^{\top} Q^{-\top / 2} \ell_{r r}^{p}\left(r^{p}\right) Q^{-1 / 2} G(\bar{\theta})+ \\
& H(\bar{\theta})^{\top} R^{-\top / 2} \ell_{r r}^{m}\left(r^{m}\right) R^{-1 / 2} H(\bar{\theta}) .
\end{aligned}
$$

When $\ell^{p}, \ell^{m}$ are least squares or Hybrid, $\mathcal{H}_{y}(\theta, y)$ is invertible for any $(\theta, y)$, and for every $\bar{\theta}$ there exist a $\bar{y}$ such that $\mathcal{H}(\bar{\theta}, \bar{y})=0$, since both penalties are strictly convex. In the case of the Student's $t$, the Hessian may fail to be positive definite at some pairs $(\theta, y)$ [3] and there is no absolute guarantee that the methodology will hold, as expected for a potentially nonconvex formulation. Practical behavior is another matter, and in numerical experience we see a positive definite Hessian at the minimizer, and so the derivative formulas hold. A safeguard can be added to any practical implementation, that can trigger a failsafe and use a less efficient method.

We now compute remaining terms in Corollary 1 , assuming for simplicity that $G(\theta)$ and $H(\theta)$ are affine functions of $\theta$.

$$
\begin{aligned}
\overline{r^{p}} & :=Q^{-\mathrm{\top} / 2} \ell_{r}^{p}\left(r^{p}\right), \quad \overline{r^{m}}:=R^{-\mathrm{\top} / 2} \ell_{r}^{m}\left(r^{m}\right) \\
f_{\theta}(\theta, \bar{y}) & =(G \bar{x})_{\theta}^{\top} Q^{-\top / 2} \ell_{r}^{p}\left(r^{p}\right)+(H \bar{x})_{\theta}^{\top} R^{-\mathrm{\top} / 2} \ell_{r}^{m}\left(r^{m}\right) \\
f_{\theta \theta}(\theta, \bar{y}) & =(G \bar{x})_{\theta}^{\top} Q^{-\top / 2} \ell_{r r}^{p}\left(r^{p}\right) Q^{-1 / 2}(G \bar{x})_{\theta} \\
& +(H \bar{x})_{\theta}^{\top} R^{-\top / 2} \ell_{r r}^{m}\left(r^{m}\right) R^{-1 / 2}(H \bar{x})_{\theta} \\
\mathcal{H}_{\theta}(\theta, \bar{y}) & =\left(G(\theta)^{\top} \overline{r^{p}}\right)_{\theta}+G(\theta)^{\top} Q^{-\top / 2} \ell_{r r}^{p}\left(r^{p}\right) Q^{-1 / 2}(G \bar{x})_{\theta} \\
& +\left(H(\theta)^{\top} \overline{r^{m}}\right)_{\theta}+H(\theta)^{\top} R^{-\top / 2} \ell_{r r}^{m}\left(r^{m}\right) R^{-1 / 2}(H \bar{x})_{\theta}
\end{aligned}
$$

We now have, fully and explicitly, first and second derivatives of the value function $v(\theta)$ in (7) for the nonsingular case. Though these results are straightforward, they do not appear in any smoothing literature we are aware of in this compact form, even for least squares losses.

## V. Singular SSM

When covariances $Q_{k}$ and $R_{k}$ are singular, we rewrite (8) to include null-space constraints. A singular covariance matrix precludes any errors and innovations that are not in its range. We follow [7] in formulating this problem:

$$
\begin{align*}
\min _{\theta, x, r^{p}, r^{m}} & \ell^{p}\left(r^{p}\right)+\ell^{m}\left(r^{m}\right) \\
\text { s.t. } & Q^{1 / 2} r^{p}=G(\theta) x-\zeta  \tag{11}\\
& R^{1 / 2} r^{m}=H(\theta) x-z
\end{align*}
$$

and introduce the Lagrangian

$$
\begin{align*}
f(\theta, y)= & \mathcal{L}\left(\theta, x, r^{p}, r^{m}, \lambda^{p}, \lambda^{m}\right) \\
= & \ell^{p}\left(r^{p}\right)+\ell^{m}\left(r^{m}\right) \\
& -\left\langle\lambda^{p}, Q^{1 / 2} r^{p}-G(\theta) x+\zeta\right\rangle  \tag{12}\\
& -\left\langle\lambda^{m}, R^{1 / 2} r^{m}-H(\theta) x+z\right\rangle .
\end{align*}
$$

When $Q_{k}$ and $R_{k}$ are invertible, we can solve for $r^{p}, r^{m}$ in (11) and reduce the problem to (8), so nonsingular systems are a special case of (11). Formulation (11) can be solved for a variety of loss functions $\ell^{p}$ and $\ell^{m}$ (see [7]).

Here we define the value function as a mini-max problem using the Lagrangian:

$$
\begin{equation*}
v(\theta):=\max _{\lambda^{p}, \lambda^{m}} \min _{x, r^{p}, r^{m}} \mathcal{L}\left(\theta, x, r^{p}, r^{m}, \lambda^{p}, \lambda^{m}\right) \tag{13}
\end{equation*}
$$

The system of equations we are interested in is now

$$
0=\mathcal{H}(\theta, y):=f_{y}(\theta, y), \quad y:=\left\{x, r^{p}, r^{m}, \lambda^{p}, \lambda^{m}\right\}
$$

that is, the system of equations that defines a saddle point of the Lagrangian. Explicitly, $f_{y}(\theta, y)=0$ is given by

$$
f_{y}(\theta, y)=\left[\begin{array}{c}
G(\theta)^{\top} \lambda^{p}+H(\theta)^{\top} \lambda^{m} \\
\ell_{r}^{p}\left(r^{p}\right)-Q^{\top / 2} \lambda^{p} \\
\ell_{r}^{m}\left(r^{m}\right)-R^{\top / 2} \lambda^{m} \\
G(\theta) x-\zeta-Q^{1 / 2} r^{p} \\
H(\theta) x-z-R^{1 / 2} r^{m}
\end{array}\right]=0
$$

$Y(\theta)$ is differentiable when $\mathcal{H}_{y}(\theta, y)=f_{y y}(\theta, y)$ is invertible:

$$
f_{y y}(\theta, y)=\left[\begin{array}{ccccc}
0 & 0 & 0 & G(\theta)^{\top} & H(\theta)^{\top}  \tag{4}\\
0 & \ell_{r r}^{p}\left(r^{p}\right) & 0 & -Q^{\top / 2} & 0 \\
0 & 0 & \ell_{r r}^{m}\left(r^{m}\right) & 0 & -R^{\top / 2} \\
G(\theta) & -Q^{1 / 2} & 0 & 0 & 0 \\
H(\theta) & 0 & -R^{1 / 2} & 0 & 0
\end{array}\right]
$$

We state the following theorem.
Theorem 2. Invertibility of $f_{y y}(\theta, y)$ is equivalent to invertibility of the so called Hessian of the Lagrangian

$$
\begin{align*}
& H(\theta) G(\theta)^{-1} Q^{1 / 2}\left(\ell_{r r}^{p}\left(r^{p}\right)\right)^{-1} Q^{\top / 2} G(\theta)^{-\top} H(\theta)^{\top} \\
& +R^{1 / 2}\left(\ell_{r r}^{m}\left(r^{m}\right)\right)^{-1} R^{\top / 2} \tag{15}
\end{align*}
$$

When $\ell^{p}, \ell^{m}$ are the least squares or Hybrid penalties, (15) is invertible if and only if

$$
\begin{equation*}
\mathcal{N}(R) \cap \mathcal{N}\left(Q G^{-T} H^{\top}\right)=\{0\} \tag{16}
\end{equation*}
$$

When Theorem 2 holds, we use Corollary (1) to get derivatives of $v(\theta)$ in 13:

$$
\begin{align*}
v(\bar{\theta}) & =f(\bar{\theta}, \bar{y}) \\
v_{\theta}(\bar{\theta}) & =f_{\theta}(\bar{\theta}, \bar{y})  \tag{17}\\
v_{\theta \theta}(\bar{\theta}) & =f_{\theta \theta}(\bar{\theta}, \bar{y})-\mathcal{H}_{\theta}(\bar{\theta}, \bar{y})^{\top} \mathcal{H}_{y}(\bar{\theta}, \bar{y})^{-1} \mathcal{H}_{\theta}(\bar{\theta}, \bar{y}) .
\end{align*}
$$

It remains only to compute $f_{\theta}, f_{\theta \theta}, \mathcal{H}_{\theta}$, and $\mathcal{H}_{y}$.

$$
f_{\theta}(\theta, \bar{y}):=\left(\left\langle\overline{\lambda^{p}}, G(\theta) \bar{x}\right\rangle\right)_{\theta}+\left(\left\langle\overline{\lambda^{m}}, H(\theta) \bar{x}\right\rangle\right)_{\theta}
$$

When $G, H$ are affine functions of $\theta$, we have $f_{\theta \theta}=0$. Finally,

$$
\mathcal{H}_{\theta}(\theta, \bar{y})=f_{y \theta}(\theta, \bar{y})=\left[\begin{array}{c}
\left(G(\theta)^{\top} \overline{\lambda^{p}}\right)_{\theta}+\left(H(\theta)^{\top} \overline{\lambda^{m}}\right)_{\theta} \\
0 \\
0 \\
(G(\theta) \bar{x})_{\theta} \\
(H(\theta) \bar{x})_{\theta}
\end{array}\right]
$$

## A. Special case: Invertible $R$.

The structural unemployment model in the introduction has a singular $Q$ but an invertible $R$. In such cases, the derivative formulas can be written using only primal quantities, which significantly decreases the notational burdern. In particular, using the optimality conditions we have

$$
\begin{aligned}
\lambda^{m} & =R^{-\top / 2} \ell_{r}^{m}\left(r^{m}\right)\left(R^{-1 / 2}(H(\theta) y-z)\right) \\
\lambda^{p} & =-G(\theta)^{-\top} H(\theta)^{\top} \lambda^{m}
\end{aligned}
$$

and so we get the explicit primal-only formula for $v_{\theta}(\theta)$ by plugging these expressions into

$$
v_{\theta}(\theta)=\left(\left\langle\overline{\lambda^{p}}, G(\theta) \bar{y}\right\rangle\right)_{\theta}+\left(\left\langle\overline{\lambda^{m}}, H(\theta) \bar{y}\right\rangle\right)_{\theta}
$$

B. Special case: Least-squares.

If $\ell^{p}(\cdot)$ and $\ell^{m}(\cdot)$ are both given by $\frac{1}{2}\|\cdot\|^{2}$, the optimality conditions simplify substantially, and we have

$$
\begin{aligned}
r^{p} & =Q^{T / 2} \lambda^{p}, \quad r^{m}=R^{T / 2} \lambda^{m} \\
Q^{1 / 2} r^{p} & =Q \lambda_{p}=G(\theta) x-\zeta \\
R^{1 / 2} r^{m} & =R \lambda_{m}=H(\theta) x-z \\
0 & =G(\theta)^{\top} \lambda^{p}+H(\theta)^{\top} \lambda^{m}
\end{aligned}
$$

Plugging these conditions back into the Lagrangian, we get the dual objective

$$
f\left(\lambda^{p}, \lambda^{m}\right)=-\frac{1}{2}\left(\lambda^{p}\right)^{\top} Q \lambda^{p}-\frac{1}{2}\left(\lambda^{m}\right)^{\top} R \lambda^{m}-\left(\lambda^{p}\right)^{\top} \zeta-\left(\lambda^{m}\right)^{\top}
$$

$$
\text { s.t. } \quad G(\theta)^{\top} \lambda^{p}+H(\theta)^{\top} \lambda^{m}=0
$$

Using invertibility of $G$, we eliminate $\lambda_{p}$ :

$$
\begin{aligned}
f\left(\lambda_{m}\right) & =-\frac{1}{2}\left(\lambda^{m}\right)^{\top}\left(H G^{-1} Q G^{-T} H^{\top}+R\right) \lambda^{m} \\
& -\left(\lambda^{m}\right)^{\top}\left(z-H G^{-1} \zeta\right)
\end{aligned}
$$

In the least squares case, the dual solution $\lambda^{m}$ is unique exactly when the linear system

$$
\begin{equation*}
H G^{-1} Q G^{-T} H^{\top}+R \tag{18}
\end{equation*}
$$

is invertible, and then we have

$$
\lambda_{m}=\left(H G^{-1} Q G^{-T} H^{\top}+R\right)^{-1}\left(z-H G^{-1} \zeta\right)
$$

a closed form solution. A simple sufficient condition for the invertibility of 18 is to have $R$ itself invertible, as in the special case previously discussed.

## VI. Numerical Examples

We now apply the results of the previous sections to analyze two simple singular models with unknown states and parameters. In Section VI-A we present a state-space formulation for the AR-1 model, show how to robustify it to outliers in the data, and present explicit derivatives for the value function. We use these derivatives to design an efficient solver for both standard and robust AR models. In Section VI-B we apply the methods in this paper to fit a structural model for unemployment rates that can track fast changes. While the structural unemployment model is currently used in the EU, in this paper we only show results on simulated synthetic data where we know ground truth, and leave any more detailed work to future collaborations.

## A. Robust AR Fitting

An AR-1 model begins with equations

$$
\begin{align*}
x_{k} & =c+\varphi x_{k-1}+\epsilon_{k}^{p}  \tag{19}\\
y_{k} & =H_{k} x_{k}+\epsilon_{k}^{m}
\end{align*}
$$

Where $\epsilon_{k}^{p}, \epsilon_{k}^{m}$ have covariances $Q_{k}, R_{k}$ respectivly, $c$ is an unknown constant, and $\varphi$ is a parameter to be estimated. To make this take the form of (1) we create an augmented state

$$
\hat{x}^{k}=\left[\begin{array}{c}
x_{k}  \tag{20}\\
c
\end{array}\right]
$$

and use state equations

$$
\begin{align*}
\hat{x}^{k} & =\left[\begin{array}{ll}
\varphi & 1 \\
0 & 1
\end{array}\right] \hat{x}_{k-1}+\hat{\epsilon}_{k}^{p} \\
y_{k} & =\left[\begin{array}{cc}
H_{k} & 0 \\
0 & 0
\end{array}\right] \hat{x}_{k}+\hat{\epsilon}_{k}^{m} \tag{21}
\end{align*}
$$

Then

$$
\begin{gathered}
\hat{Q}_{0}=\left[\begin{array}{cc}
Q_{0} & 0 \\
0 & 1
\end{array}\right], \quad \hat{Q}_{k}=\left[\begin{array}{cc}
Q_{k} & 0 \\
0 & 0
\end{array}\right] \quad k>0 \\
\hat{R}_{k}=\left[\begin{array}{cc}
R_{k} & 0 \\
0 & 0
\end{array}\right]
\end{gathered}
$$

This choice of $\hat{Q}_{0}$ will allow us to fit the constant $c$ as ${ }^{\top} p_{Z}$ art of the state while $\hat{Q}_{k}, k>0$ will act as equality constraints holding it constant through all time points. In order to compute the derivatives of the value functions we first note the following derivative formula in this case for any vector $\eta$.

$$
\left(G_{i}(\theta) \eta\right)_{\theta}=\left(\left[\begin{array}{ll}
\varphi & 1  \tag{22}\\
0 & 1
\end{array}\right]\left[\begin{array}{l}
\eta^{1} \\
\eta^{2}
\end{array}\right]\right)_{\theta}=\left[\begin{array}{c}
\eta^{1} \\
0
\end{array}\right]=\tilde{D} \eta
$$

Where $\tilde{D}=\left[\begin{array}{ll}1 & 0 \\ 0 & 0\end{array}\right]$. Define

$$
D=\left[\begin{array}{cccc}
0 & 0 & & \\
\tilde{D} & 0 & \ddots & \\
& \ddots & \ddots & 0 \\
& & \tilde{D} & 0
\end{array}\right]
$$

Then using the above, for the AR-1 model

$$
(G(\theta) x)_{\theta}=-D x
$$

And similarly

$$
\left(G(\theta)^{T} \lambda\right)_{\theta}=-D^{\top} \lambda
$$

We now have the expressions

$$
\begin{gathered}
f_{\theta}(\theta, \bar{y}):=-\left\langle\overline{\lambda^{p}}, D \bar{x}\right\rangle \\
f_{\theta \theta}=0 \\
\mathcal{H}_{\theta}(\theta, \bar{y})=-\left[\begin{array}{c}
D^{\top} \overline{\lambda^{p}} \\
0 \\
0 \\
D \bar{x} \\
0
\end{array}\right]
\end{gathered}
$$

When combined with the general results of section $\bar{V}$, we get

$$
\begin{align*}
v(\bar{\theta}) & =f(\bar{\theta}, \bar{y}) \\
v_{\theta}(\bar{\theta}) & =f_{\theta}(\bar{\theta}, \bar{y})=-\left\langle\overline{\lambda^{p}}, D \bar{x}\right\rangle  \tag{23}\\
v_{\theta \theta}(\bar{\theta}) & =-\mathcal{H}_{\theta}(\bar{\theta}, \bar{y})^{\top} \mathcal{H}_{y}(\bar{\theta}, \bar{y})^{-1} \mathcal{H}_{\theta}(\bar{\theta}, \bar{y}) .
\end{align*}
$$

## B. Fast Tracking of Unemployment Rates

In this section, we apply the proposed approach to estimate parameters $\left(\ell_{1}, \ell_{2}, \gamma\right)$ for the structural unemployment model (2) - (4). To test the approach, we generate ground truth parameters and then create synthetic data in order to compare model performance and speed using different formulations and algorithms. The data is generated by fixing parameters to reasonable values similar to those observed in practice, namely at $\left[\begin{array}{lll}\ell_{1} & \ell_{2} & \gamma\end{array}\right]=\left[\begin{array}{lll}0.68 & 1.41 & -0.68\end{array}\right]$, and applying the unemployment rate state space model (2) - (4) to generate the state as well as noisy observations. We then consider three cases: nominal errors, outliers in the observations, and jumps in the unemployment process. In the nominal cases we use variance parameters known to the smoother. To generate outliers we randomly select $10 \%$ of measurements and add additional noise drawn from a $\mathcal{N}(0,1)$ Gaussian distribution. To generate large jumps we add large deviations $.4,-.2$ at indices corresponding to 25 and 65. To Examples of the generated data are in Figure 2 An example of the estimated using this data are in Figure 3 .
All algorithms are initialized at $\left[\begin{array}{lll}0 & 0 & 0\end{array}\right]$, except for LMNewton on $T / l \mathrm{l}$ in the nominal case, which is initialized at $\left[\begin{array}{lll}0 & 0 & 0.5\end{array}\right]$, as the standard zero initialization leads to bad results for this (nonconvex) case.

In the first iteration the state is initialized by propagating the initial $x_{0}$ through the dynamics for all time. In subsequent iterations the state is always initialized using the previous state solution. In all methods, the full state at each iteration is computed using Newton's method to find a saddle point of the augmented Lagrangian

$$
\begin{align*}
A L(y, \theta)= & \ell^{p}\left(r^{p}\right)+\ell^{m}\left(r^{m}\right) \\
& -\left\langle\lambda^{p}, Q^{1 / 2} r^{p}-G(\theta) x+\zeta\right\rangle \\
& -\left\langle\lambda^{m}, R^{1 / 2} r^{m}-H(\theta) x+z\right\rangle  \tag{24}\\
& +\frac{1}{2}\left\|Q^{1 / 2} r^{p}-G(\theta) x+\zeta\right\|^{2} \\
& +\frac{1}{2}\left\|R^{1 / 2} r^{m}-H(\theta) x+z\right\|^{2}
\end{align*}
$$

using the Hessian of the Lagrangian provided in the Appendix.
The value at an optimal point of 24 is the same as at an optimal point of 12 . 24, is better conditioned which leads to faster convergence in practice. For the outer iterations on the parameter space we compare a Newton method, LBFGS, and a LM-Newton solver. The standard Newton and L-BFGS are from a standard python library. The LM-Newton solver is a quasi-Newton method where the Hessian is boosted by a parameter that is updated adaptively based on model performance. The results are summarized in Table I

All methods work well for convex models. In the nonconvex case, the algorithms become more sensitive. In particular when $\ell^{p}$ is student's T , we have to boost $\ell_{r r}^{p}$ by a constant in order


Fig. 2: Example of generated data with outliers (top) and large jumps (bottom). Observations are shown in gray.
to make Newtons method converge. In practice this constant must be tuned depending on the parameter $\nu$ in the student's T function. Convergence is therefore sensitive to the choice of $\nu$ and boosting constant but a good rule of thumb is to choose $1 \leq \nu \leq 20$ and boost just enough to make the Hessian positive semidefinite.

## VII. DISCUSSION

We presented a general approach for parameter estimation in singular and non-singular Kalman smoothing models. In particular we showed how to compute first and second derivatives of the value function (optimizing over state) with respect to the hidden parameters for both singular and nonsingular cases, which captures a wide variety of models, including the motivating example. A simple numerical illustration shows how the computed quantities can be used by a variety of optimization methods. The examples also show that when working with structural parameters, it pays off to have convex subproblems within each iteration of the value function. While non-convex losses such as Student's $t$ are always appealing from a modeling perspective, when the problem is to find both the state and parameters, the resulting models are more fragile than those that use convex losses. This observation opens the way to future research in both theory and algorithm design.

|  |  | Nominal |  |  | Outliers |  |  | Large Jumps |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | 1s/ls | T/ls | H/ls | 1s/ls | 1s/T | 1s/H | 1s/ls | T/ls | H/ls |
| Newton | $\\|\hat{\theta}-\theta\\|^{2}$ | 0.158 | 0.143 | 0.1884 | 1.72 | 0.115 | 0.142 | 0.296 | 0.032 | 0.099 |
|  | Inner Iter | 19 | 250 | 206 | 14 | 71 | 102 | 21 | 329 | 373 |
|  | Outer Iter | 9 | 5 | 10 | 6 | 15 | 13 | 13 | 9 | 14 |
|  | Time | 11.5 | 36.5 | 29.7 | 6.3 | 20.2 | 19.3 | 13.3 | 48.1 | 49.5 |
| L-BFGS | $\\|\hat{\theta}-\theta\\|^{2}$ | 0.158 | 0.137 | 0.184 | 1.72 | 0.115 | 0.141 | 0.296 | 0.034 | 0.099 |
|  | Inner Iter | 19 | 228 | 207 | 19 | 86 | 88 | 32 | 375 | 519 |
|  | Outer Iter | 10 | 18 | 10 | 9 | 17 | 12 | 16 | 14 | 15 |
|  | Time | 6.2 | 33.9 | 26.5 | 6.3 | 19.4 | 14.0 | 10.6 | 51.4 | 67.5 |
| LM-Newton | $\\|\hat{\theta}-\theta\\|^{2}$ | 0.158 | $0.069{ }^{11}$ | 0.184 | 1.04 | 0.12 | 0.142 | 0.296 | 0.028 | 0.099 |
|  | Inner Iter | 16 | 385 | 180 | 32 | 70 | 114 | 24 | 302 | 357 |
|  | Outer Iter | 12 | 15 | 20 | 25 | 28 | 19 | 18 | 15 | 21 |
|  | Time | 7.2 | 51.6 | 26.4 | 14.4 | 20.0 | 21.0 | 11.3 | 43.2 | 48.1 |

TABLE I: Table of results when run on generated data. The second row indicates the loss functions that were used where is stands for least squares $\left(\frac{1}{2}\left\|\|^{2}\right)\right.$, T stands for Students T with $\nu=10$, and H stands for Hybrid with $\epsilon=.7$.


Fig. 3: Example of estimated solution run on data in Figure 2 Top is 1s/H run on data with outliers. Bottom panel shows T/ls run on data with large jumps added. Both are computed using Newton's method.
was supported by the Boeing Data Science Research Grant.

## REFERENCES

[1] B. D. Anderson and J. B. Moore. Optimal control: linear quadratic methods. Courier Corporation, 2007.
[2] B. D. O. Anderson and J. B. Moore. Optimal Filtering. Prentice Hall, 1979.
[3] A. Y. Aravkin, J. V. Burke, and G. Pillonetto. Robust and trend-following student's t kalman smoothers. SIAM Journal on Control and Optimization, 52(5):2891-2916, 2014.
[4] Y. Bar-Shalom, X. Rong Li, and T. Kirubarajan. Estimation with applications to tracking and navigation. John Wiley \& Sons, Inc., New York, 2001.
[5] B. M. Bell and J. V. Burke. Algorithmic differentiation of implicit functions and optimal values. In Advances in Automatic Differentiation, pages 67-77. Springer, 2008.
[6] R. J. Hyndman, A. B. Koehler, R. D. Snyder, and S. Grose. A state space framework for automatic forecasting using exponential smoothing methods. International Journal of Forecasting, 18(3):439-454, 2002.
[7] J. Jonker, A. Aravkin, J. V. Burke, G. Pillonetto, and S. Webster. Fast robust methods for singular state-space models. Automatica, 105:399405, 2019.
[8] H. N. Mocan. Structural unemployment, cyclical unemployment, and income inequality. Review of Economics and Statistics, 81(1):122-134, 1999.
[9] R. S. Tsay. Analysis of financial time series, volume 543. John Wiley \& Sons, 2005.

Acknowledgment. We are very grateful to Jon Nielsen (Economic Council of the Labour Movement (ECLM)) for pointing us to the use of Kalman smoothers in structural unemployment models, and for teaching us about these models. Research of A. Aravkin and P. Zheng was supported by the Washington Research Foundation Data Science Professorship. J. Jonker

## Appendix

a) Proof of Theorem 2. We reduce $\mathcal{H}_{\mathcal{X}}(\theta, \mathcal{X})$ in 14 to block upper triangular form using invertible block row operations

$$
\begin{aligned}
& \mathcal{R}_{1}=\left(\ell_{r r}^{p}\left(r^{p}\right)\right)^{-1} \mathcal{R}_{1} \\
& \mathcal{R}_{2}=\left(\ell_{r r}^{m}\left(r^{m}\right)\right)^{-1} \mathcal{R}_{2} \\
& \mathcal{R}_{3}=G(\theta)^{-T} \mathcal{R}_{3} \\
& \mathcal{R}_{4}=-G(\theta)^{-1}\left(\mathcal{R}_{4}-Q^{1 / 2} \mathcal{R}_{1}-Q^{1 / 2}\left(\ell_{r r}^{p}\left(r^{p}\right)\right)^{-1} Q^{T / 2} \mathcal{R}_{3}\right) \\
& \mathcal{R}_{5}=\mathcal{R}_{5}-R^{1 / 2} \mathcal{R}_{2}-H \mathcal{R}_{4}
\end{aligned}
$$

The resulting system is given by

$$
\left[\begin{array}{ccccc}
I & 0 & -\left(\ell_{r r}^{p}\right)^{-1} Q^{T / 2} & 0 & 0 \\
0 & I & 0 & 0 & -\left(\ell_{r r}^{m}\left(r^{m}\right)\right)^{-1} R^{T / 2} \\
0 & 0 & I & 0 & -G^{-1} H^{\top} \\
0 & 0 & 0 & I & G^{-1} Q^{1 / 2}\left(\ell_{r r}^{p}\left(r^{p}\right)\right)^{-1} Q^{T / 2} G^{-T} H^{\top} \\
0 & 0 & 0 & 0 & \left(H G^{-1} Q^{1 / 2}\left(\ell_{r r}^{p}\left(r^{p}\right)\right)^{-1} Q^{T / 2} G^{-T} H^{\top}\right. \\
& & & & \left.+R^{1 / 2}\left(\ell_{r r}^{m}\left(r^{m}\right)\right)^{-1} R^{T / 2}\right)
\end{array}\right]
$$

The invertibility of $\mathcal{H}_{\mathcal{X}}$ is thus equivalent to the invertibility of the symmetric positive semidefinite system (15).
b) Hessian of the Lagrangian 24):

$$
A L_{y y}(y, \theta)=\left[\begin{array}{ccccc}
G(\theta)^{T} G(\theta)+H(\theta)^{T} H(\theta) & -G(\theta)^{T} Q^{1 / 2} & -H(\theta)^{T} R^{1 / 2} & G(\theta)^{T} & H(\theta)^{T}  \tag{25}\\
-Q^{T / 2} G(\theta) & \ell_{r r}^{p}\left(r^{p}\right)+Q^{T / 2} Q^{1 / 2} & 0 & -Q^{T / 2} & 0 \\
-R^{T / 2} H(\theta) & 0 & \ell_{r r}^{m}\left(r^{m}\right)+R^{T / 2} R^{1 / 2} & 0 & -R^{T / 2} \\
G(\theta) & -Q^{1 / 2} & 0 & 0 & 0 \\
H(\theta) & 0 & -R^{1 / 2} & 0 & 0
\end{array}\right]
$$


[^0]:    *Department of Mathematics, University of Washington, Seattle, WA (jonkerjo@uw.edu)
    ${ }^{\dagger}$ Department of Applied Mathematics, University of Washington, Seattle, WA (zhengp@uw.edu)
    ${ }^{\dagger}$ Department of Applied Mathematics, University of Washington, Seattle, WA (saravkin@uw.edu)

