Innovations in Likelihood-Based Inference for State Space Models

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1. Introduction

There are several terms that have been used as synonyms with state space models (SSMs):

- Mechanistic model
- Hidden Markov model (HMM)
- Partially observed Markov process (POMP) model

I chose SSM as it is the terminology often preferred by practitioners.

I Follow the definition used by Durbin and Koopman (2012) for a SSM.

- Let $Y_1, Y_2, \ldots, Y_N$ be random variable representing the observed time series. These observations occur at time points $t_1, \ldots, t_N$, and can be vector valued.
- A SSM introduces unobservable (latent) states $X_1, \ldots, X_N$ at the same observation times. These latent variables are connected to the observations, in a way defined by the model.

I will adopt the shorthand $t_{1:N} = (t_1, \ldots, t_N)$, $Y_{1:N} = (Y_1, \ldots, Y_N)$, and $X_{1:N} = (X_1, \ldots, X_N)$.

When defining a SSM, we often want to include an initial value for the latent states, X_0.

We assume that the random variables $Y_{1:N}$, $X_{0:N}$ have a joint probability density $f_{X_{0:N}, Y_{1:N}}(x_{0:N}, y_{1:N}; \theta)$ with respect to some dominating measure (typically Lebesgue or a counting measure), where θ is a parameter vector $\theta \in \mathbb{R}^{d_\theta}$ that indexes the model.

The difficulty in likelihood-based inference for these models is a result of only $Y_{1:N}$ being observable, and thus the likelihood function involves a high-dimensional integral:

$$\mathcal{L}(\theta; y^*) = f_{Y_{1:N}}(y_{1:N}^*; \theta) = \int f_{X_{0:N}, Y_{1:N}}(x_{0:N}, y_{1:N}^*; \theta) \, dx_{0:N}. \tag{1}$$

A common approach is to treat SSMs as partially observed Markov process (POMP) models. We make the following assumptions:

- We assume that the latent variables are a Markov process

$$f_{X_n|X_{1:n-1}}(x_n|x_{1:n-1}; \theta) = f_{X_n|X_{n-1}}(x_n|x_{n-1}; \theta).$$

- Measurements are conditionally independent

$$f_{Y_n|X_{1:N},Y_{-n}}(y_n|x_{0:N}, y_{-n}; \theta) = f_{Y_n|X_n}(y_n|x_n; \theta).$$

With these assumptions, we can express the joint density as

$$f_{X_{0:N},Y_{1:N}}(x_{0:N}, y_{1:N}; \theta) = f_{X_0}(x_0; \theta) \prod_{n=1}^{N} f_{X_n|X_{n-1}}(x_n|x_{n-1}; \theta) f_{Y_n|X_n}(y_n|x_n; \theta). \tag{2}$$
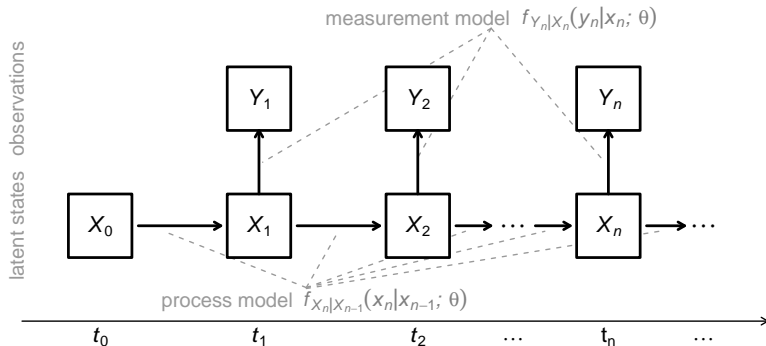
Figure 1: A flow diagram representing an arbitrary POMP model. Modified figure from SBIED course (King, Ionides).

Each of the SSMs considered in this thesis are POMP models.

Other common terms that are sometimes used as synonyms are used for special cases

Mechanistic Model

A SSM (or POMP) where the evolution of latent variables is dictated by equations mimicing real-world mechanisms.

Hidden Markov Model (HMM)

A SSM (or POMP) where the latent variables take values in a discrete and finite space.

- Inference for ARMA models.
- Mechanistic models for modeling cholera outbreak in Haiti.
- The marginalized panel iterated filter (MPIF) algorithm.

2. Likelihood Maximization for ARMA models

Auto-regressive moving average (ARMA) models

ARMA models are the most frequently used approach to modeling time series data. ARMA models are as foundational to time series analysis as linear models are to regression analysis, and they are often used in conjunction for regression with ARMA errors.

ARMA model definition

A time series $Y_{1:N}$ is called ARMA(p, q) if it is (weakly) stationary and

$$Y_n = \phi_1 Y_{n-1} + \cdots + \phi_p Y_{n-p} + w_n + \varphi_1 w_{n-1} + \ldots + \varphi_q w_{n-q}, \tag{3}$$

with $\{w_n; n = 0, \pm 1, \pm 2, \ldots\}$ denoting a mean zero white noise (WN) processes with variance $\sigma_w^2 > 0$, and $\phi_p \neq 0$, $\varphi_q \neq 0$.

We refer to the positive integers p and q of Eq. (3) as the autoregressive (AR) and moving average (MA) orders, respectively.

For practitioners, ARMA models do not appear to be SSMs. However, inference methodology treats ARMA models as *non-mechanistic* SMMs. Let $r = \max(p, q + 1)$, and we now define

$$X_n = \begin{pmatrix} Y_n \\ \phi_2 Y_{n-1} + \ldots + \phi_r Y_{n-r+1} + \varphi_1 w_n + \ldots + \varphi_{r-1} w_{n-r+2} \\ \phi_3 Y_{n-1} + \ldots + \phi_r Y_{n-r+2} + \varphi_2 w_n + \ldots + \varphi_{r-1} w_{n-r+3} \\ \vdots \\ \phi_r Y_{n-1} + \varphi_{r-1} w_n \end{pmatrix} \in \mathbb{R}^r$$

$$T = \begin{pmatrix} \phi_1 & 1 & 0 & \ldots & 0 \\ \phi_2 & 0 & 1 & \ldots & 0 \\ \vdots & \vdots & & \ddots & \\ \phi_{r-1} & 0 & \ldots & & 1 \\ \phi_r & 0 & \ldots & & 0 \end{pmatrix} \in \mathbb{R}^{r \times r}, \qquad Q = \begin{pmatrix} 1 \\ \varphi_1 \\ \vdots \\ \varphi_{r-1} \in \mathbb{R}^r \end{pmatrix}$$

We can then recover the ARMA model using the following state space formulation:

$$X_n = TX_{n-1} + Qw_n$$
$$Y_n = \begin{pmatrix} 1 & 0 & \dots & 0 \end{pmatrix} X_n$$

This results in a linear-Gaussian SSM, and the likelihood function $\mathcal{L}(\theta)$ can be evaluated exactly using the Kalman filter (Kalman, 1960).

- The likelihood can be maximized by combining this with a numeric optimizer (Gardner et al., 1980).

This approach has been the standard method for fitting ARIMA models since the early 2000's due to modern computing capabilities (Ripley, 2002).

This existing approach frequently results in sub-optimal parameter estimates. To demonstrate this, we fit an $\mathrm{ARMA}(2,2)$ and an $\mathrm{ARMA}(2,1)$ model to data generated from an $\mathrm{ARMA}(2,2)$ model. The $\mathrm{ARMA}(2,1)$ is formally a special case of an $\mathrm{ARMA}(2,2)$ model, with $\varphi_2 = 0$.

In **R**, we draw a single instance from Model class 2: $y^*_{1:100} \sim \mathrm{ARMA}(2,2)$ with:

- $(\phi_1, \phi_2, \varphi_1, \varphi_2) = (0.2, -0.1, 0.4, 0.2)$
- $w_n \overset{\text{iid}}{\sim} N(0,1)$.
- Intercept $\mu = 13$ so that $E[Y_n] \neq 0$.

The Gardner et al. (1980) is the standard method for fitting ARMA model parameters. It is implemented in the base **stats** package in R, as well as the **statsmodels** module in Python.

```
mod1 <- stats::arima(y, order = c(2, 0, 1))
mod2 <- stats::arima(y, order = c(2, 0, 2))
```

The likelihood of **mod1** is -141.2, and the likelihood of **mod2** is -144.3. The smaller model has a log-likelihood that is 3.1 units higher than the larger model, which is mathematically impossible under proper optimization.

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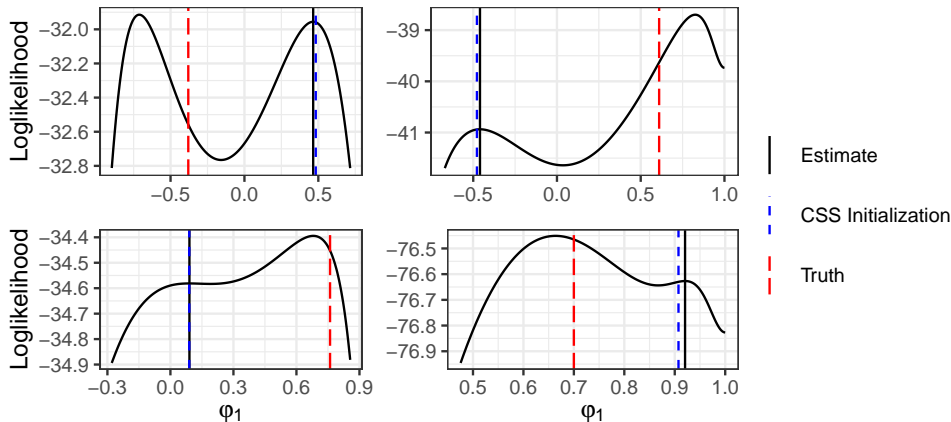
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The difficulty is that the likelihood surface is often multimodal, and the existing procedure runs the risk of converging to a local solution (Ripley, 2002).

In other contexts with multi-model loss functions, the optimization is often repeated using multiple initializations. However, I have seen no instances of this for ARIMA models. There are a few challenges:

- Most users don't know about the possibility of converging to local solutions.
- Their are complex constraints of possible initialization.
  - Constraints are on the roots of polynomials formed by model parameters, not directly on parameters themselves.

The roots of the polynomials $\Phi(x) = 1 - \phi_1 x - \phi_2 x^2 - \ldots - \phi_p x^p$ and $\Psi(x) = 1 + \varphi_1 x + \varphi_2 x^2 + \ldots + \varphi_q x^q$ must lie outside the complex unit circle.

Multiple parameter initializations

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For parameters to be real, the roots need to be sampled as real or conjugate pairs. We cannot sample all roots as conjugate pairs (or real), as this would result in specific parameters being all one sign. Our approach for each root is the following:

- Sample inverted-root magnitudes uniformly $U(\gamma, 1 - \gamma)$.
- With probability $p = \sqrt{1/2}$, sample inverted-root pairs as real.
  - ▶ If real, assign the same sign with probability p.
  - ▶ If complex, sample angle from $U(0, \pi)$, and use to assign conjugate pairs of inverted-roots.
- With roots sampled, calculate corresponding coefficients and perform optimization routine.
- Repeat until convergence.

Now we'll fit the exact same models using the **arima2** package:

```
mod1v2 <- arima2::arima(y, order = c(2, 0, 1))
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With this new algorithm and software, the likelihood of **mod1v2** is -141.2, and the likelihood of **mod2v2** is -141.2.

The likelihood of the smaller model was unchanged, but the larger model had an increase in log-likelihood of 3.1. The likelihoods of the nested models are now consistent.

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ARMA models are not necessarily state-of-the art statistical models. Why does this project matter?

- ARMA models are among the most frequently used approaches in all of statistics, so even small improvements are worth the effort.
- Software that claims to maximize model likelihoods fails to do so in a large number of cases ($> 20\%$).
- ARMA models are often used in conjunction with linear regression. Likelihood ratio tests are common for testing the inclusion / significance of regression parameters.
  - Typical improvements in log-likelihood in the range $(0.22, 1.46)$. This shortcoming in one or both model is large enough to change the outcome of these tests.
- Even if outcomes are unchanged, confidence that software / algorithms will reliably do what you expect is important.

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3. Informing Policy via Dynamic Models: Cholera in Haiti

One of the most scientifically interesting types of SSMs are *mechanistic models.*

- Used when we have some understanding of how a dynamic system evolves over time.
- Useful in modern science, and have some advantages over machine learning models (Baker et al., 2018; Hogg and Villar, 2024):
  - ▶ Accounting for known (but unobserved) features can improve model performance.
  - ▶ More intepretable.
  - ▶ Facilitates predictions of interventions and other counter-factuals.

In this chapter, I demonstrate these capabilities by fitting mechanistic models to the 2010-2019 cholera outbreak in Haiti (Wheeler et al., 2024).

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- Haiti experienced a cholera outbreak following the devastating 2010 earthquake.
- From 2010-2019, more than 800,000 recorded cases, making it one of the largest recorded outbreaks.
- Oral cholera vaccination (OCV) is available, but in limited supply.
- Image credit: UNICEF (2022).

A group of top researchers built three mechanistic models to estimate the potential impacts of various vaccination strategies (Lee et al., 2020).

- The distinct teams each concluded predicted cholera resurgence from Feb 2019 - Feb 2024.
- There were no confirmed cases from Feb 2019 - Sep 2022 (Trevisin et al., 2022).
- Though there were some cases recently recorded, not near the predicted scale (Pan American Health Organization, 2023).

Questions: What are strengths and weaknesses of mechanistic models? What are common mistakes researchers make? How can we improve outcomes in the future?
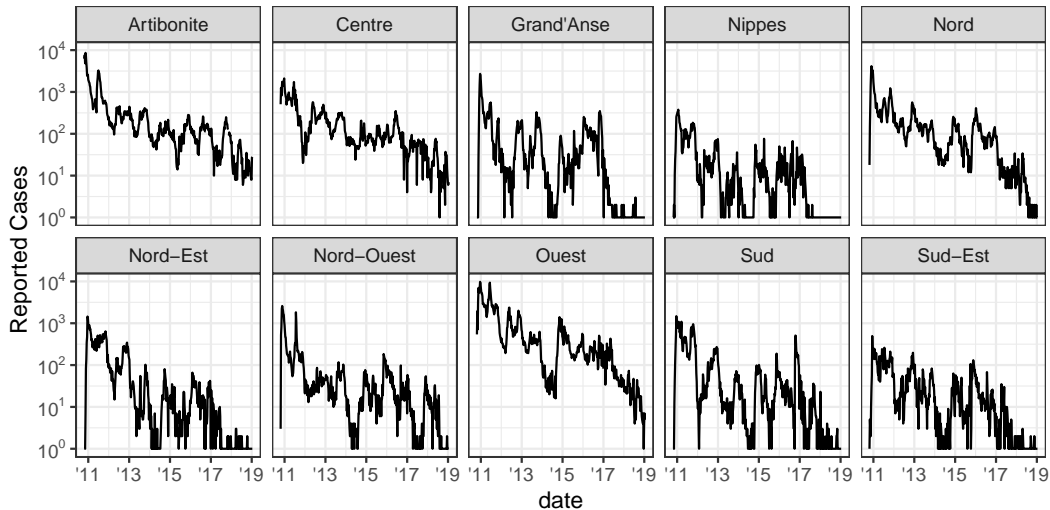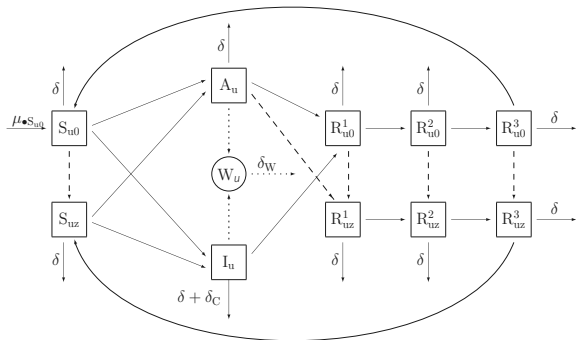
- Spatial Dependence between units.
- Stochastic transmission rates.
- Overdispersed Markov counting system.
- Rainfall driven transmission.
- Environmental reservoir of bacteria.
- Adjustments for Hurricane Mathew (Oct 2016).

The iterated block particle filter (IBPF) was used to fit the model (Ionides et al., 2024).

	Our Fit	Original Fit	Benchmark
Log-likelihood	-17332.9	-33832.6	-17932.6
AIC	34733.9	67723.2	35945.0

Table 1: Comparison of our fitted model to original parameters used to inform vaccination policy.

Key findings

- Confirmed importance of rainfall and reduced transmission over time.
- Importance of proper model diagnostics.
  - ▶ Comparing to benchmarks.
  - ▶ Checking results against features of the system.
- Reproducibility and Extendability.
- Confirmed previous findings: stochastic models are better descriptions of the system, and over-dispersed models are best.

4. The Marginalized Panel Iterated Filter (MPIF)

Often we have a collection of related time series called, called *panel data*. We want to make inference using the entire collection, not just on each time series.

Examples

- Model for disease outbreaks of the same disease, different locations (hospitals / cities) (Lee et al., 2020).
- Experiments / observational studies on ecological populations (Searle et al., 2016).
- Longitudinal studies using within-host dynamic models (Ranjeva et al., 2017).

Mechanistic models are routinely fitted to time series data but seldom to panel data, despite its widespread availability.

Measurements for unit u taken at times $t_{u,1:N_u}$. Observed and latent process at these times denoted $Y_{u,n}$ and $X_{u,n}$, respectively.

Each unit u defines an independent POMP model, the entire collection of models is a PanelPOMP.

$$\mathcal{L}(\theta; y^*) = \int \prod_{u=1}^{U} f_{X_{u,0}}(x_{u,0}; \theta) \prod_{n=1}^{N_u} f_{X_{u,n}|X_{u,n-1}}(x_{u,n}|x_{u,n-1}; \theta) f_{Y_{u,n}|X_{u,n}}(y_{u,n}|x_{u,n}; \theta) dx_{1:U,0:N_u}.$$

The parameter vector θ has shared components ϕ, and unit specific components $\psi_{1:U}$.

$$\theta = (\phi, \psi_{1:U})$$

.

- Particle filters work in low-dimensions, can be applied independently to units.
- Iterated filtering (IF) is an extension used to perform maximum likelihood estimation (Ionides et al., 2015).
- IF introduces dependence because of shared θ, making it a high-dimensional problem.

IF is a special type of Data cloning (Lele et al., 2007), which is repeated applications of Bayes rule.

Denote $\pi_i(\theta)$ as the posterior distribution of the parameter vector θ after the ith Bayesian update, and $\mathcal{L}(\theta; \mathbf{y}^*)$ as the likelihood

$$\pi_1(\theta) \propto \mathcal{L}(\theta; \mathbf{y}^*)\pi_0(\theta),$$
$$\pi_2(\theta) \propto \mathcal{L}(\theta; \mathbf{y}^*)\pi_1(\theta) \propto \mathcal{L}(\theta; \mathbf{y}^*)^2\pi_0(\theta),$$
$$\vdots$$
$$\pi_m(\theta) \propto \mathcal{L}(\theta; \mathbf{y}^*)^m\pi_0(\theta).$$

If we let $m \to \infty$, the effect of the initial prior distribution diminishes, and the mth posterior has all of its mass centered at the MLE.

Loosely speaking, iterated filtering is just data cloning with the additional pieces:

1. Likelihood cannot be evaluated exactly, it's approximated using particle filters.
2. At each time-step, the parameter particles are perturbed.
3. Parameter particles reweighted using conditional log-likelihoods.

The perturbation of parameters is necessary to avoid particle depletion, a known problem with particle filters + Bayesian inference (Chen et al., 2024).

The perturbations introduce a loss of information (Liu, 2001), so are decreased over the cloning iteration.

The panel iterated filter (PIF) is a type of IF, mitigating information loss (Bretó et al., 2020). It has been successfully used to estimate the MLE previously (e.g., Domeyer et al., 2022).

Theorem (Chapter 4, Theorem 1)

Extends theory of Chen et al. (2024) to panel models. Denote the output of the PIF algorithm as $\Theta_{1:J}^{(M)}$. Then there exists some positive sequences $\{C_M\}_{M \geq 1}$ and $\{\epsilon_M\}_{M \geq 1}$ where $\lim_{M \to \infty} \epsilon_M = 0$ such that for all $(J, M) \in \mathbb{N}^2$,

$$E\left[\left|\left|\frac{1}{J}\sum_{i=1}^{J}\Theta_j^{(M)} - \hat{\theta}\right|\right|_2\right] \leq \frac{C_M}{\sqrt{J}} + \epsilon_M$$

Conditions:

- On parameter space Θ: Compact, corners not too "sharp" (regular compact set, Def 1 of Chen et al., 2024).
- Regularity conditions on the model (positive and finite likelihood, densities are smooth functions of θ).
- Conditions on the parameter perturbations (type of perturbations, and cooling schedule).

Proof Sketch:

- Chen et al. (2024) provides framework for convergence of IF of POMP models; we write a general PanelPOMP as a POMP model, and PIF is a special case of IF for these models.

Iterated filtering takes data one observation at a time. In the panel setting, this means we process by unit u. Ignoring perturbations, the algorithm iterates over (m, u):

$$\pi_{m,u}(\theta) \propto \mathcal{L}_u(\theta; y_u^*)\, \pi_{m,u-1}(\theta) = \mathcal{L}_u(\phi, \psi_u; y_u^*)\, \pi_{m,u-1}(\theta), \tag{4}$$

Using $\pi_{0,0}(\theta)$ as the initial prior distribution. Even if prior is independent, we get dependence by iterating Eq. 4 over u. Two options of iterated filtering:
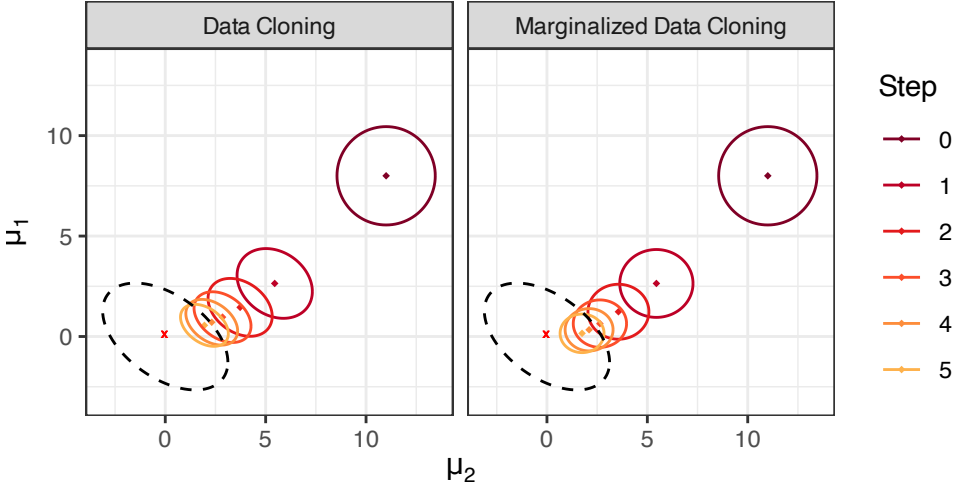
- Perturb all parameters at each time step (high loss of information).
- When using data from unit u, only perturb ϕ and ψ_u (the PIF algorithm, high particle depletion).

If the last prior $\pi_{m,u-1}(\theta)$ has independence: $\pi_{m,u-1}(\theta) = f(\psi_{-u})g(\phi, \psi_u)$, then there is no need to resample particles ψ_{-u}. This would avoid the particle depletion *and* loss-of-information.

This leads to marginalized data cloning (repeating Eqs. 5–6).

$$\tilde{\pi}_{m,u}(\theta) \propto \mathcal{L}_u(y_u^*; \phi, \psi_u)\, \pi_{m,u-1}(\theta) \tag{5}$$

$$\pi_{m,u}(\theta) \propto \int \tilde{\pi}_{m,u}(\theta)\, d\phi\, d\psi_u \times \int \tilde{\pi}_{m,u}(\theta)\, d\psi_{-u}. \tag{6}$$

- Like IF extends data cloning, the MPIF algorithm extends this marginalized data cloning.

- Existing theory for IF algorithms cannot readily be extended to MPIF, because of the non-linearity introduced by the marginalization step.

- A natural first question is whether or not marginalized data cloning converges.

  ▶ Unfortunately, a few toy examples suggests not always.

Convergence is explored via Gaussian likelihoods. The properties of this special case is relevant to the broader class of models that is well approximated by Gaussian models, (e.g., local asymptotic normality (Le Cam and Yang, 2000)).

Theorem (Chapter 4, Theorem 2)

Let $\mathcal{L}_u(y_u^*; \phi, \psi_u)$ be the likelihood that corresponds to a Gaussian distribution with mean (ϕ^*, ψ_u^*) and precision $\Lambda_u^* \in \mathbb{R}^{2 \times 2}$. Under suitable conditions on the matrices Λ_u^*, then if the initial prior density is Gaussian, then the density of the mth iteration of Eq. 6 converges to a point mass at the MLE $(\phi^*, \psi_1^*, \ldots, \psi_U^*)$ as $m \to \infty$.

- Gaussian priors + Gaussian likelihoods imply Gaussian posteriors.
- Transform data so likelihood is centered at zero.
- The marginalization step only modifies the covariance, setting off-diagonal terms to zero.
- Diagonals of covariance shrink to zero asymptotically at rate $1/m$.
- Each unit-iteration updates the ϕ and ψ_u components of μ_m.
- $\mu_m = \left(\prod_{i=1}^{m} \prod_{u=1}^{U} A_{u,i} \right) \mu_0 = \left(\prod_{i=1}^{m} P_m \right) \mu_0$, with $\|P_m\|_2 = 1 - \epsilon_m/m + o(1/m)$, with ϵ_m positive, bounded.

5. Concluding Remarks

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Section 6

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