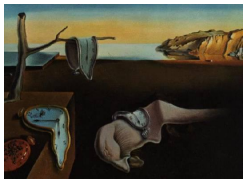

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pypomp: Inference for partially observed Markov process models in Python with JAX DRAFT IN PROGRESS

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Abstract

—!!!—an abstract is required—!!!—

Keywords: —!!!—at least one keyword is required—!!!—.

1. Introduction

[Topic]

Partially Observable Markov Process (POMP) models, also known as state-space models or hidden Markov models, provide a flexible and mechanistic framework for modeling time-series

dynamic systems, particularly suited for scenarios where latent states are only partially observable. Characterized by transition densities and measurement densities of Markov processes, this framework bridges complex underlying dynamics with limited information in real-world data. Consequently, POMP models find extensive application in epidemiology (Mietchen, Clancey, McMichael, and Lofgren 2024; Fox, Lachmann, Tec, Pasco, Woody, Du, Wang, Ingle, Javan, Dahan, Gaither, Escott, Adler, Johnston, Scott, and Meyers 2022; Wen, Yin, Li, Peng, and He 2024), ecology (Auger-Méthé, Newman, Cole, Empacher, Gryba, King, Leos-Barajas, Mills Flemming, Nielsen, Petris, and Thomas 2021; Marino, Peacor, Bunnell, Vanderploeg, Pothoven, Elgin, Bence, Jiao, and Ionides 2019; Blackwood, Streicker, Altizer, and Rohani 2013), finance (Bretó 2014), and other domains.

[Existing package discussion]

The POMP package ecosystem in `R` has provided a solid, standardized, and extensible framework for modeling time series data using nonlinear, stochastic partially observed mechanism dynamic models. The `R pomp` package has become a well-established tool for fitting POMP models using a general and abstract representation, that supports multiple inference techniques. Its extension packages `panelPomp`, `spatpomp`, and `phyloPomp` further enhance its capabilities for panel, spatio-temporal, and phylodynamic data analysis, respectively.

[computational challenges + potential limitations]

While conceptually powerful, statistical inference for POMP models using the above `R` packages poses substantial computational challenges. From a methodological perspective, likelihood-based inference for POMP models typically relies on perturbations within iterated filtering (adding ref related to iterative filtering) algorithms. While many of them are stable and effective in locating a neighborhood containing the likelihood maximum, they exhibit numerical inefficiency for obtaining a precise identification of the maximum value. Particularly, when the latent states are high-dimensional or when repeated model evaluations are required, the fitting process could be computationally prohibitive by the constraints.

As it turns out, POMP methods can be sped up considerably. Many of the processes involved in POMP methods are embarassingly parallel, such as simulating the state process for each of thousands of particles, running the particle filter multiple times for the same parameter set, and running iterated filtering from multiple starting parameter sets, especially when estimating a profile likelihood to construct a confidence interval as per (Ionides, Breto, Park, Smith, and King 2017). Graphics Processing Units (GPUs) are well-suited for such operations. However, the existing family of POMP packages (**pomp**, **panelPomp**, and **spatPomp** (King, Nguyen, and Ionides 2016, Bretó, Wheeler, King, and Ionides (2025), Asfaw, Park, King, and Ionides (2024))) only runs on CPUs.

[introducing AD/JIT/GPU hardware + pypomp]

As the demand grows for scalable and parallelizable inference algorithms, there is an increasing need for an accelerated framework for POMP modeling framework. The Python package `pypomp` (Abkemeier, Chen, Ionides, Wheeler, and Tan 2024) addresses this by integrating **automatic differentiation (AD)**, **just-in-time (JIT) compilation**, and **GPU acceleration** through JAX (Bradbury, Frostig, Hawkins, Johnson, Leary, Dougal Maclaurin, Necula, Paszke, VanderPlas, Skye Wanderman-Milne, and Zhang 2018), a high-performance numerical computing library that supports hardware acceleration and vectorization. AD techniques

enable efficient and accurate derivative computation by systematically applying the chain rule to fundamental operations. Recent works have extended AD for gradient estimation using particle filtering, yielding a class of methods termed automatic differetiation particle filters (ADPF). Building on these advancements, `pypomp` provides AD-enabled gradient estimation for inference for POMP models within a plug-and-play framework (Ionides, Breto, and King 2006), where users specify dynamic models solely through simulators of latent state trajectories, rather than evaluating the transition density of the latent Markov process. JAX's JIT compilation further accelerates repeated inference and evaluation by converting Python functions into machine code at runtime. Finally, JAX's GPU support enables efficient scaling of inference methods. Together, these features make `pypomp` more than a port of the `R` package `pomp`. Instead, it establishes an independent, modernized platform for fast and flexible POMP modeling in Python.

[structure]

The remainder of this paper is organized as follows. Section 2 discusses the motivation for `pypomp` design using specific examples. Section 3 demonstrates the mathematical notation for POMP models and their related implementation in `pypomp`. Section 4 introduces the embedded methodologies. Section 5 presents data analysis workflows and benchmarking results. Section 6 concludes with a discussion of future directions.

[add discussion of panelpomp into introduction]

2. Motivation for pypomp

[This section is for some extra detailed numeric cost estimates and dataset descriptions to illustrate motivation based on Aaron's draft. It is a bit redundant now.]

2.1. Real-world computational bottleneck

Computational speed is a major bottleneck in the practical application of iterated filtering methods to POMP models. In Korevaar, Metcalf, and Grenfell (2020) 's dataset, fitting and evaluating likelihoods of POMP models for 180 units required 8 days on 36 CPU cores (two 3.0 GHz Intel Xeon Gold 6154 CPUs). Scaling this up to the full dataset of 1422 units would require almost eight times as much effort, equivalent to running 36 cores for two months or 288 cores for 8 days. This is not only time consuming, but also incurs substantial computational costs, highlighting the urgent need for more efficient inference software for large-scale POMP analyses Importantly, this cost only accounts for one round of iterated filtering. In practice, to further refine the likelihood estimates, multple rounds are required, which would increase the computational burden significantly. This motivates the development of accelerated, scalable tools to make large-scale POMP inference feasible.

2.2. Opportunities for speeding up the POMP models

Many of the processes involved in fitting POMP models are embarrassingly parallel. Examples include simulating the state process for each of thousands of particles, running the particle filter repeatedly under the same parameter set, and executing iterated filtering from

multiple starting parameter sets. Such parallelism is especially advantageous when estimating a profile likelihood to construct confidence intervals (Ionides *et al.* 2017). Harnessing parallel computing resources can therefore dramatically reduce computation time and make large-scale inference feasible.

Graphics Processing Units (GPUs) are well-suited for embarrassingly parallel operations, but the existing family of POMP packages (**pomp**, **panelPomp**, and **spatPomp** (King *et al.* 2016, Bretó *et al.* (2025),Asfaw *et al.* (2024))) are limited to CPU computation. None provide support for GPU acceleration or automatic differentiation. These two technologies are key to enabling scalable and efficient inference for modern POMP applications.

2.3. Our solution: pypomp

To address this computational bottleneck, we are creating `pypomp`(Abkemeier *et al.* 2024), a python implementation of the `R` package `pomp`. It draws inspiration from `pomp`, but further implements new methods incoporating automatic differentiation techniques by forking the source code used in Tan (Tan, Hooker, and Ionides 2024), as well as leverages JAX's just-in-time(JIT) compilation and GPU core parallelization (Bradbury *et al.* 2018), allowing practitionersto run filtering methods significantly faster and cheaper. For example, in an SPX comparison model, we show that, compared to `pomp` with 36 CPU cores, `pypomp` can run at least 7 times faster and can finish the job at 5% of the price using 1 GPU and 1 CPU core (5120 CUDA cores on a NVIDIA Tesla V100 and one core from a 2.4 GHz Intel Xeon Gold 6148 CPU).

In addition, `pypomp` is gradually including functionality from `panelPomp` and `spatPomp`, offering a unified Python interface for entire POMP methodologies across multiple `R` packages. It also takes advantage of JAX's implementation of automatic differentiation (AD), which can be used in conjunction with the differentiable measurement off-parameter with discount factor α (MOP-α) particle filter to improve local optimization of the likelihood surface (Tan *et al.* 2024).

2.4. Summary of key features

Table 1 summarizes the main differences between `pypomp` and `pomp`, highlighting the new capabilities of `pypomp`.

Feature	pypomp	pomp
Backend and Acceleration	JAX (GPU/CPU, JIT,`vmap`, `jax.grad`, `jax.Hessian`)	R and C Snippets (CPU only)
Automatic Differentiation and gradient-based inference	Yes (gradient/Hessian via AD supported)	No
Particle Filtering Methods	Yes (PF, MOP-α, IF2, IFAD)	Yes (PF, IF2, pMCMC, etc.)
Plug-and-Play Property	Yes	Yes

Object Design	In-place updates on current objects, stored in the object attribute `results_history`	Returns new objects

Table 1: Feature comparison between `pypomp` and `pomp` in R ecosystem.

3. POMP Models in pypomp

This section introduces the structure of POMP models and its implementation in `pypomp`, including both mathematical setup and the package implementation.

3.1. Model setup

A **partially observed Markov process (POMP)** model has two main components: (i) a latent Markov process that evolves over time and (ii) an observation process that links the latent states. Together, these jointly specify the mechanistic model for the observed time series, providing a framework for modeling dynamic systems where measurements are noisy. Formally, suppose we observe the process at discrete time $n = 1, \dots, N$, with initial time 0. Let $Y_{1:N}$ denote the observations and $X_{0:N}$ denote the corresponding latent (unobserved) Markov process at the corresponding time. A POMP model is defined by three building components, each corresponding to user-supplied Python functions in `pypomp`:

1. initial density: $f_{X_0}(x_0;\theta)$, implemented via `rinit`, generates draws of the initial states X_0.
2. transition density: $f_{X_n|X_{n-1}}(x_n \mid x_{n-1};\theta)$, implemented via `rproc`, propagates the evolution of latent states.
3. measurement density: $f_{Y_n|X_n}(y_n \mid x_n;\theta)$, implemented via `dmeas`, evaluates or simulates observations conditional on the latent states.

Here, we hold an conditional independence assumption that, given X_n, the observation Y_n is independent of all other variables. Then, the joint density of $(X_{0:N}, Y_{1:N})$ can be expressed as the product of the initial distribution, the transition densities, and the measurement densities:

$$f_{X_{0:N},Y_{1:N}}(x_{0:N}, y_{1:N};\theta) = f_{X_0}(x_0;\theta)\prod_{n=1}^{N} f_{X_n|X_{n-1}}(x_n \mid x_{n-1};\theta)\prod_{n=1}^{N} f_{Y_n|X_n}(y_n \mid x_n;\theta)$$

The marginal likelihood of the observations is $\mathcal{L}(\theta) = f_{Y_{1:N}}(y_{1:N};\theta) = \int f_{X_{0:N},Y_{1:N}}(x_{0:N}, y_{1:N};\theta)\, dx_{0:N}$. In practice, this integral is intractable for most nonlinear or non-Gaussian POMP models, motivating the use of simulation-based inference methods such as particle filtering.

3.2. Implementations of POMP models in pypomp

Object-oriented interface

A POMP model in `pypomp` is represented as an object of class `Pomp`, which encapsulates the model components: the initial state distribution, process model, and measurement model. This object-oriented interface allows users to specify by passing components to the constructor, including observations, model parameters, model mechanics such as simulators and the measurement density, covariates, and times. After the components are passed into the constructor, the constructor automatically generates additional internal elements, such as extended observations and covariates required for interpolation

Table 2 summarizes the main arguments to the Pomp constructor and their correspondence to mathematical objects. `RInit`, `RProc` and `RMeas` are the subconstructors, where they specify the stochastic mechanisms that define a `Pomp` model, and their objects are passed as arguments when initializing a main `Pomp` class.

Constructor/Sub-constructor	Argument	Type	Description / Mathematical representation
Pomp	`rinit`	`RInit`	simulate initial states $X_0 \sim f_{X_0}(x_0;\theta)$
	`rproc`	`RProc`	simulate state transitions $X_n \sim f_{X_n\|X_{n-1}}(x_n \mid x_{n-1};\theta)$
	`rmeas`	`RMeas`	simulate observations $Y_n \sim f_{Y_n\|X_n}(y_n \mid x_n;\theta)$
	`dmeas`	`DMeas`	evaluate measurement density $f_{Y_n\|X_n}(y_n \mid x_n;\theta)$
	`ys`	`pandas.DataFrame`	observations $y^*_{1:N}$ with times $t_{1:N}$
	`covars`	`pandas.DataFrame`	covariates $z^*_{1:N}$ with times $s_{1:N}$
	`theta`	`list` or `dict`	parameters θ
RInit	`t0`	`float`	initial time point t_0 for simulation
RProc	`step_type`	`str`	method of process evolution: `"fixedstep"` or `"euler"`
	`nstep`	`int`	number of steps if `step_type="fixedstep"`
	`dt`	`float`	time step if `step_type="euler"`
	`accumvars`	`tuple`	indices of state variables to be accumulated
RMeas	`ydim`	`int`	observation dimension $\dim(Y)$

Table 2: Main arguments to the `Pomp` class and related constructor objects.

We demonstrate here how to create a `Pomp` object. Specifically, we show how to create the linear Gaussian model included in the package as `LG()`. We begin by importing necessary packages and defining helper functions for handling the parameters. Because `pypomp` will run our defined model components within JAX JIT-compiled code, it is necessary to write the components to be JAX-compliant. Naturally, the JAX package has many useful functions for this purpose. We also generate a pseudorandom number generation (PRNG) key to be used with JAX random number generators. All stochastic simulations in `pypomp` are controlled via JAX PRNG keys, ensuring full reproducibility when using the same seed.

```
import pypomp as pp
import pandas as pd
import jax
import jax.numpy as jnp
from functools import partial


def get_thetas(theta):
    theta = jnp.asarray(theta)
    A = theta[0:4].reshape((2, 2))
    C = theta[4:8].reshape((2, 2))
    Q = theta[8:12].reshape((2, 2))
    R = theta[12:16].reshape((2, 2))
    return A, C, Q, R


def transform_thetas(A, C, Q, R):
    return jnp.concatenate([A.ravel(), C.ravel(), Q.ravel(), R.ravel()])


key = jax.random.key(1)
```

Model Components

We refer to model components describing initialization, transfer, or measurement processes as model mechanisms, including `rinit`, `rproc`, `dmeas`, and `rmeas`. Users must define these processes as Python functions. Specifically, we require users to provide function code to the object constructor, which verifies that all necessary function arguments are included and in the correct order. This requirement stems from `pypomp`'s internal mechanism: it vectorizes component functions using `jax.vmap()` to efficiently run thousands of particles. Since `jax.vmap()` maps functions to input arrays by position rather than keyword, users must strictly adhere to parameter order. While all expected parameters must be included, the function does not need to utilize all of them.

Illustrated in Table 2,`pypomp` also includes object constructors for components describing the model mechanics: `RInit`, `RProc`, `DMeas`, and `RMeas`. Some constructors also require additional arguments, such as `t0` for `RInit`. Notably, `RProc` takes `step_type`, `dt`, and `nstep` arguments. `step_type` determines how `RProc` should be run at intermediate steps between two observation times. If we want to model the state process as evolving in continuous time, setting `step_type="euler"`uses an Euler approximation, running `rproc` at intermediate steps based on the time step size, `dt`. The number of steps taken is given by the number of times `dt` divides the difference between two observation times, rounded up, and is consequently dynamic. Otherwise, if we instead want a fixed number of steps for each observation time interval, we can use `step_type="fixedstep"`, in which case `rproc` will run at `nstep` intermediate steps equally spaced between two observation times, starting from the first observation time. Consequently, setting `step_type="fixedstep"` and `nstep=1` only runs `rproc` at the observation times. Here is an example of defining the object constructors for components under the lin-

ear gaussian model.In practice, at least one of `dmeas` or `rmeas` must be provided, while the construction of `RInit` and `RProc` are always required.

```
import pypomp as pp

@partial(pp.RInit, t0=0.0)
def rinit(theta_, key, covars=None, t0=None):
    A, C, Q, R = get_thetas(theta_)
    return jax.random.multivariate_normal(key=key, mean=jnp.array([0.0, 0.0]), cov=Q)

@partial(pp.RProc, step_type="fixedstep", nstep=1)
def rproc(X_, theta_, key, covars=None, t=None, dt=None):
    A, C, Q, R = get_thetas(theta_)
    return jax.random.multivariate_normal(key=key, mean=A @ X_, cov=Q)

@pp.DMeas
def dmeas(Y_, X_, theta_, covars=None, t=None):
    A, C, Q, R = get_thetas(theta_)
    # return logpdf of Y given X (mean = C @ X_, cov = R)
    return jax.scipy.stats.multivariate_normal.logpdf(Y_, mean=C @ X_, cov=R)

@partial(pp.RMeas, ydim=2)
def rmeas(X_, theta_, key, covars=None, t=None):
    A, C, Q, R = get_thetas(theta_)
    return jax.random.multivariate_normal(key=key, mean=C @ X_, cov=R)
```

Parameters

The `Pomp` constructor also requires model parameters. These can be provided either as a dictionary or as a list of dictionaries. Each item in a dictionary should include the parameter name as the key and the parameter value as the dictionary value. If the parameter sets are provided as a list of dictionaries, methods such as `pfilter()` run on each set of parameters. Here, we use `Pomp.sample_params()` to sample sets of parameters from uniform distributions with bounds passed as a dictionary of length-2 tuples. `Pomp.sample_params()` returns a ready-to-use list of dictionaries with the sampled parameters. Internally, parameters, even are multi-dimensional, are stored as flat dictionaries to facilitate JAX transformations and compilation.

```
theta = {
    "A11": jnp.cos(0.2), "A12": -jnp.sin(0.2),
    "A21": jnp.sin(0.2), "A22": jnp.cos(0.2),
    "C11": 1.0, "C12": 0.0, "C21": 0.0, "C22": 1.0,
    "Q11": 0.01, "Q12": 1e-6, "Q21": 1e-6, "Q22": 0.01,
    "R11": 0.1, "R12": 0.01, "R21": 0.01, "R22": 0.1,
}
param_bounds = {k: (v * 0.9, v * 1.1) for k, v in theta.items()}
n = 5
```

```
key = jax.random.PRNGKey(1)
key, subkey = jax.random.split(key)
theta_list = pp.Pomp.sample_params(param_bounds, n, subkey)
```

3.3. Covariates

Scientifically, POMP models often involve external time-varying inputs, referred to as covariates, which can influence either the latent process or the measurement model. Examples include seasonality, interventions, or environmental drivers in ecological applications. In `pypomp`, covariates are supplied as a `pandas.DataFrame` indexed by time. The time at which the covariates were observed should be specified in the `ctime` argument. Importantly, the covariate time points may differ from the observation times, necessitating interpolation. Given the observation times, covariate times, and the step type specified in `RProc`, the model automatically aligns and interpolates observations and covariates to ensure consistency with the simulation of the latent and observation processes. The linear gaussian model doesn't involve any covariates, and an example using covariates is given in the Data Analysis Section.

POMP Object Construction

We do not have real data in this `LG` example, so we generate our own. To make this example cleaner, we here use the function `LG()` to construct the completed linear Gaussian model object and then generate the data using `simulate()`. Observation times are provided to the `Pomp` constructor via the `pandas.DataFrame` row index. If covariates were provided, the times at which the covariates were observed would also be provided by the `pandas.DataFrame` row index.

```
import jax, jax.numpy as jnp
import pandas as pd
import pypomp as pp

T = 100
# ensure `key` exists; if not, uncomment the next line
# key = jax.random.PRNGKey(1)

key, subkey = jax.random.split(key)
sims = pp.LG(T=T).simulate(key=subkey)

ys = pd.DataFrame(
    sims[0]["Y_sims"].squeeze(),
    index=range(1, T + 1),
    columns=["Y1", "Y2"],
)

LG_obj = pp.Pomp(
    rinit=rinit,
    rproc=rproc,
    dmeas=dmeas,
```

```
    rmeas=rmeas,
    ys=ys,
    theta=theta_list,
    covars=None,
)

print("LG_obj created; ys.shape =", ys.shape)
```

Each argument to `Pomp` is accessible from the object as an attribute.

```
print(LG_obj.rinit) # access POMP model components
print(LG_obj.rproc)
print(LG_obj.dmeas)
print(LG_obj.rmeas)
print(LG_obj.theta)   # access parameters
print(LG_obj.ys.head())  # access observations
```

Premade models:

Beyond the linear gaussian model, `pypomp` includes several ready-to-use model constructors that serve both as examples and as tested templates for custom model development:

1. `LG()` — a simple linear-Gaussian model with 2-dimensional latent and observed states; useful to validate API usage and diagnostics.
2. `spx()` — the S&P500 log-return model from Sun et al. (Sun 2024).
3. `dacca()` — the cholera transmission model from King et al. (King, Ionides, Pascual, and Bouma 2008).
4. `UKMeasles.Pomp()` — the measles district model from He et al. (He, Ionides, and King 2010), wired to the Korevaar et al. dataset (Korevaar *et al.* 2020). Panel and spatial variants (PanelPOMP/SpatPOMP style) are planned.

These examples show correct component wiring (`rinit`, `rproc`, `dmeas`, `rmeas`), recommended `step_type`/`dt` usage, and typical diagnostics. If a user model errors or runs slowly, compare its components to the matching premade model to find mistakes and performance opportunities. Meanwhile, these premade models can also replicate well-know case studies in the R pomp ecosystem, allowing direct comparison and validation.

JAX Numerical Backend and Interface Design

A key design choice `pypomp` is it relys heavily on the JAX numerical backend. Unlike the R package `pomp`, where users typically provide POMP model components in C Snippets for acceleration, `pypomp` requires model components to be written as JAX-compatible Python functions. These functions are then compiled and vectorized by JAX tools such as `jit` and `vmap`. This design leads to several important interface features:

- **Strict argument requirements for compilation and vectorization:** JAX's `jit` compiler transforms the user-supplied component functions (`rinit`, `rproc`, `dmeas`, `rmeas`) into efficient machine code, while `vmap` efficiently run them over thousands of particles via vectorization of arguments. To ensure the compatibility with JAX's

compilation and vectorization system, each component function must follow the expected input types and order, otherwise compilation would fail.

- **PRNG random key policy**: To ensure the reproducibility of randomness in POMP models under `pypomp`, the public API accept an optional `jax.random.PRNGkay`, which is explicityly passed through constructors and methods. Keys are internally split when it is needed. Unlike the R setting, where randomness can be controlled globally or by seed chunks, in JAX, random keys only be explicitly passed through funcitons
- **Consistent shapes and sizes handling**: model parameters, even multidimensional, are stored as flattened dictionaries. Consequently, JAX can uniformly process parameters, thereby maintaining consistency in particle propagation.

Later section will demonstrate how the JAX-based design supports further inference methods.

[more introduction to JAX?]

Panel POMP class

4. POMP Methods in pypomp

In this section, we describe the core inference methods currently implemented in `pypomp`, including :

- `Paricle Filter` (Sequential Monte Carlo, written in `pfilter()`): A standard sequential Monte Carlo algorithm for likelihood evaluation and state estimation, forming the basis for most inference methods in POMP models.
- `Differentiated Measurement-off-policy` Particle Filter (MOP(α), written in `mop()`): A recently proposed SMC method (Tan *et al.* 2024) that evaluates the likelihood at one parameter value while obtaining resampling decisions from another, adjusting via discounted off-parameter measurement weights.
- `Iterated Filtering` (IF2, `mif()`): A classical IF2 algorithm (Ionides, Nguyen, Atchadé, Stoev, and King 2015) for likelihood-based parameter inference that maximizes the likelihood via particle filtering.
- `Iterated Filtering with Automatic Differentiation` (`train()`): A recently proposed AD-based algorithm (Tan *et al.* 2024) that incorporates MOP(α), the differentiable particle filter, to enable efficient gradient-based parameter inference for maximum likelihood estimation.

A key feature of the above POMP inference methods lies in the **plug-and-play property** (Ionides *et al.* 2006), meaning that inference algorithms can be implemented without requiring explicit evaluation of the transition density of the latent process. Instead, it suffices for the user to provide a simulator of the latent process (`rproc`), initial state distribution (`rinit`), and observation measurement model (`dmeas`, `rmeas`). This property enables POMP methods to be widely applied to complex mechanistic models where transition densities are intractable.

In `pypomp`, the plug-and-play design is fully preserved: users only need to provide component functions compliant with JAX requirements, which can be directly plugged in inference

methods like `pfilter()`, `mop()`, `mif()`, and `train()`. The package combines the generality of plug-and-play modeling with the efficiency of JAX compilation and vectorization.

Unlike the R family of POMP packages, some `Pomp` class methods including `pfilter()`, `mif()` and `train()` yield results by modifying the object in place instead of returning new objects. All of results are stored a list under `LG_obj.results_history`, which is an attibute under `Pomp` class object `LG_obj`. Each element in the list correponds to one method call. Each element includes results such as the log-likelihood and parameter estimates when applicable as well as the inputs used for the function call, so it is easy to keep track of how the results were calculated. If multiple parameter sets are supplied in a list as an argument, the method evaluates at each set and the results for each are stored. Meanwhile, each following method in `pypomp` that takes a key as an argument stores an unused child key under `LG_obj.fresh_key` that later method calls can use by default when a key argument is not given. This design prevents repeated use of the same key across a sequence of method calls and ensures proper randomness.

```
LG_obj.pfilter(J = 100,
               reps = 5,
               key = subkey)
LG_obj.mif(sigmas = 0.02,
           sigmas_init = 0.1,
           M = 2,
           a = 0.5,
           J = 100,
           key = subkey)

print(LG_obj.results_history)
```

4.1. Particle Filter (pfilter)

[outline: 1. purpose/role 2. implementation details in pypomp 3. outputs/results 4. remarks/highlights]

The particle filter algorithm (sequential Monte Carlo, SMC) (Arulampalam, Maskell, Gordon, and Clapp (2002), King *et al.* (2016)) is the core classical likelihood evaluation tool in POMP model inference. It uses Monte Carlo techniques to sequentially estimate the integrals in the prediction and filtering recursions, and produce an unbiased Monte Carlo estimate of the likelihood of the observed data under a parameter set. The likelihood estimate is essential for other parameter inference algorithms such as iterative filtering. In `pypomp`, the basic particle filter is implemented under `pfilter()`. The algorithm is summarized as Algorithm 1,

Algorithm 1 Sequential Monte Carlo (SMC, or particle filter) in textttpypomp: `LG_obj.pfilter(J=J, reps=reps, key=key)`, where `LG_obj` is a class `Pomp` object with components `rinit`, `rproc`, `dmeas`, `rmeas`, `ys`, and `theta`

Require Simulator for $\text{process}_n(\cdot|x_n;\theta)$; Evaluator for $f_{Y_n|X_n}(y_n \mid x_n;\theta)$; Simulator for $f_{X_0}(x_0;\theta)$; Parameter θ; Data $y^*_{1:N}$; Number of particles J.

Initialize particles: $X^{F,\theta}_{0,j} \sim f_{X_0}(\cdot;\theta)$ for $j = 1{:}J$.

For $n = 1, ..., N$:

Simulate prediction particles: $X^{P,\theta}_{n,j} \sim \text{process}_n(\cdot|x_n;\theta)$ for $j = 1{:}J$.

Evaluate weights and measurement density: $w(n,j) = f_{Y_n|X_n}(y^*_n \mid X^{P,\theta}_{n,j};\theta)$ for $j = 1{:}J$.

Normalize weights $\tilde{w}(n,j) = \dfrac{w(n,j)}{\sum_{m=1}^{J} w(n,m)}$ for $j = 1:J$.

Select resample indices $k_{1:J}$ with $P(k_j = m) = \tilde{w}(n,m)$.

Obtain resampled particles $X^{F,\theta}_{n,j} = X^{P,\theta}_{n,k_j}$ for $j = 1{:}J$.

Compute conditional log likelihood:

$$\hat{\ell}_{n|1:n-1} = \log\left(\frac{1}{J}\sum_{m=1}^{J} w(n,m)\right).$$

Return Log likelihood estimate $\hat{\ell}(\theta) = \sum_{n=1}^{N} \hat{\ell}_{n|1:n-1}$; filter samples $X^{F,\theta}_{n,1:J}$ for $n = 1{:}N$.
Complexity: $\mathcal{O}(J)$

In `pypomp`, the `pfilter()` functions is internally run in a compiled JAX routine `pfilter_internal()` but wrapped up into a class method. `_pfilter_internal` is JIT-compiled with static arguments, in which the replicates and parameter sets are vectorized via `jax.vmap`. Both techniques enable execution on CPU/GPU and ensure the computational efficiency. In implementation, the weights and likelihood are stored in a log scale, preventing underflow. There are optional arguments (`CLL`, `ESS`, `filter_mean`, `prediction_mean`) control wheter additional diagnostic arrays are allocated and updated. The algorithm works for flexible and extendable models through the user-specified `Pomp` class components (`rinit`, `rproc`, `dmeas`, `reams`), number of particles `J` as well as other parameters. Each run returns a `dict` type element updated inside the `LG_obj. result_history` attribute, containing the log-likelihoods, algorithm parameters used, as well as model diagonostic elements at each time included if their respective boolean flags are set to True. For example, suppose we run

```
LG_obj_2 = pp.Pomp(
    rinit=rinit,
    rproc=rproc,
    dmeas=dmeas,
    rmeas=rmeas,
    ys=ys,
    theta=theta_list,
    covars=None,
)
```

```
LG_obj_2.pfilter(J = 1000,
                 reps = 10,
                 key = subkey)

LG_obj_2.pfilter(J = 1000,
                 reps = 10,
                 key = subkey,
                 CLL = True,
                 ESS = True,
                 filter_mean = True,
                 prediction_mean = True)
```

where J is the number of particles used and *reps* is the number of particle filtering replicates to run for each parameter set provided in the `Pomp` object or as an optional argument to `pfilter()`. Because `LG_obj2.result_history` begins as an empty list here when the model is constructed, the results are appended at `LG_obj_2.results_history[0]` and `LG_obj_2.results_history[1]` respectively. Both of these two dictionaries contain with the following items:

- `method`: The method that was run. In this case, `pfilter`.
- `logLiks`: An `xarray.DataArray` of particle filter log-likelihood estimates. There is one list for each parameter set given and each list has `reps` log-likglihood estimates. dimensions = (`theta`, `replicate`)
- `theta`: The list of parameter sets used.
- `J`: The number of particles used.
- `thresh`: Threshold value for resampling used, which is 0 by default.

Meanwhile, `LG_obj_2.results_history[1]` also contains the following items that are not contained in `LG_obj_2.results_history[0]` :

- `CLL`: An `xarray.DataArray` containing the conditional loglikelihood over observed time steps (`theta`, `replicate`, `time`)
- `ESS`: An `xarray.DataArray` containing the effective sample size over observed time steps (`theta`, `replicate`, `time`)
- `filter_mean`: An `xarray.DataArray` containing the filtered mean over observed time steps (`theta`, `replicate`, `time`, `state`)
- `prediction_mean`: An `xarray.DataArray` containing the prediction mean over observed time steps. (`theta`, `replicate`, `time`, `state`)

A key design is that all runs across multiple parameter sets and replications are stored in one `results_history` list under the corresponding `Pomp` object. This avoids object duplication, and increases reproducibility by facilitating pickling `Pomp` objects obtained from many different search strategies, loading them into a new Python session, and then comparing the results to see how they vary with different algorithmic parameters.

4.2. Differentiated Measurement Off-Parameter (DMOP) particle filter

([TO BE REWRITTEN, FOLLOWING ISSUE 2])

[Motivation for DMOP] Classical particle filters for POMP models produce unbiased Monte Carlo estimates, but are non-differentiable in model parameters θ, due to the discrete random sampling of particles. This prevents the wide use of AD and gradient-based optimization in POMP dynamical systems. The differentiable measurement off-parameter particle filter (DMOP-α, Tan *et al.* (2024)) provides a solution: it treats a *differentiable* likelihood estimator produced by a variant of the standard particle filter as an objective and apply AD to obtain $\nabla_\theta \widehat{\ell}(\theta)$ for likelihood-based optimal parameter search. The derivative estimate from DMOP-α is essential for further stochastic gradient inference methods, such as iterated filtering with automatic differentiation (IFAD), where it employs stochastic gradient descent using DMOP-α. A tunning dicount factor $\alpha \in [0, 1]$ controls the bias-variance trade-off of the gradient estimator: larger α may result in lower bias and higher variance, while smaller α can reduce the variance with the cost of increasing bias. In implementation, DMOP-α does not require heavy diagnostics or multiple replicates. It only needs a stable, differentiable of the (log-) likelihood to feed into `jax.grad` and `jax.value_and_grad`. The pseudocode is shown in 2

Algorithm 2 DMOP-α in `pypomp`: `jax.value_and_grad(LG_obj.mop(J=J, reps=reps, key=key, alpha=alpha))`. `LG_obj` is a `Pomp` object with components `rinit`, `rproc`, `dmeas`, `ys`, `theta`.

Require Simulator process$_n(\cdot|x_n;\theta)$; Evaluator for $f_{Y_n|X_n}(y_n^*|x_n,\theta)$; Simulator for $f_{X_0}(\cdot;\theta)$; Evaluation parameter θ; Data $y_{1:N}^*$; Number of particles J; Discount factor α.

Initialize particles $X_{0,j}^{F,\theta} \sim f_{X_0}(\cdot\,;\,\theta)$, weights $w_{0,j}^{F,\theta} = 1$ for $j = 1:J$.

For $n = 1, ..., N$:

Simulate prediction particles, $X_{n,j}^{P,\theta} \sim \text{process}_n(\,\cdot\,|X_{n-1,j}^{F,\theta};\theta)$ for $j = 1:J$.

Accumulate discounted prediction weights, $w_{n,j}^{P,\theta} = (w_{n-1,j}^{F,\theta})^{\alpha}$.

Evaluate measurement density, $g_{n,j}^{\theta} = f_{Y_n|X_n}(y_n^*|X_{n,j}^{P,\theta}\,;\,\theta)$ for $j = 1:J$.

Compute conditional likelihood in version B: $L_n^{B,\theta,\alpha} = \sum_{j=1}^{J} g_{n,j}^{\theta}\, w_{n,j}^{P,\theta} \,/\, \sum_{j=1}^{J} w_{n,j}^{P,\theta}$.

Select resampling indices $k_{1:J}$ with $P(k_j = m) \propto g_{n,m}^{\theta}$.

Obtain resampled particles $X_{n,j}^{F,\theta} = X_{n,k_j}^{P,\theta}$.

Calculate corrected weights $w_{n,j}^{F,\theta} = w_{n,k_j}^{P,\theta}\, g_{n,k_j}^{\theta} \,/\, \texttt{stop\_gradient}(g_{n,k_j}^{\theta})$.

Compute considtional likelihood in version A: $L_n^{A,\theta,\alpha} = L_n^{\phi} \cdot \sum_{j=1}^{J} w_{n,j}^{F,\theta} \,/\, \sum_{j=1}^{J} w_{n,j}^{P,\theta}$.

Forward Pass: AD constructs a computation graph to evaluate the likelihood estimate $\hat{L}^A(\theta) = \prod_{n=1}^{N} L_n^{A,\theta,\alpha}$ or $\hat{L}^B(\theta) = \prod_{n=1}^{N} L_n^{B,\theta,\alpha}$.

Backward Pass: AD propagates gradients through the computation graph and evaluates gradient estimate $\hat{\mathcal{D}}^A(\theta)$ or $\hat{\mathcal{D}}^B(\theta)$

Return: likelihood estimate $\hat{L}^A(\theta)$ or $\hat{L}^B(\theta)$, and gradient estimate $\hat{\mathcal{D}}^A(\theta)$ or $\hat{\mathcal{D}}^B(\theta)$.

The key building block of the DMOP-α is the MOP-α algorithm, a variant of the standard particle filter designed to make the discontinuous Monte Carlo resampling process independent of the target parameter θ. It evaluates the likelihood at the evaluation parameter θ but draws resampling indices using weights computed at another baseline behavior parameter ϕ. This renders the likelihood estimates differentiable w.r.t. θ, further enabling AD.

In DMOP-α, the same idea is implemented equivalently by setting $\phi \equiv \texttt{stop\_gradient}(\theta)$ in JAX. This prevent its input from being differentiated. The filtering process therefore runs

$\theta = \phi$, assuming the evaluation parameter and the bahavior parameters have identical values. This avoids the need to explicitly introduce new parameters while preserving the differentiable property. Consequently, the likelihood evaluation of DMOP is identical to that of the standard particle filter, and it does not require implement a fully separate MOP-α procedure. This design simplifies the algorithm and still ensures the valid likelihood and gradient estimator, while maintaining differentiability with respect to θ. That is, DMOP computes the derivative of the likelihood estimate obtained by MOP when $\theta = \phi$. The pseudocode of MOP is shown in 3.

Algorithm 3 MOP(α), Measurement off-policy sequential Monte Carlo

Require Simulator for process$_n(\cdot|x_n;\theta)$; Evaluator for $f_{Y_n|X_n}(y_n \mid x_n;\theta)$; Simulator for $f_{X_0}(x_0;\theta)$; Evaluation Parameter θ; Behavior Parameter ϕ; Data $y^*_{1:N}$; Number of particles J.

Initialize filter particles $X^{F,\theta}_{0,j} \sim f_{X_0}(\cdot;\theta)$ and $w^{F,\theta}_{0,j} = 1$ for $j = 1{:}J$.

For $n = 1, ..., N$:

Simulate prediction particles: $X^{P,\theta}_{n,j} \sim f_{X_n|X_{n-1}}(\cdot \mid X^{F,\theta}_{n-1,j};\theta)$ for $j = 1{:}J$.

Accumulate discounted Prediction weight: $w^{P,\theta}_{n,j} = \left(w^{F,\theta}_{n-1,j}\right)^{\alpha}$ for $j = 1{:}J$.

Evaluate measurement density: $g^{\theta}_{n,j} = f_{Y_n|X_n}(y^*_n \mid X^{P,\theta}_{n,j};\theta)$ for $j = 1{:}J$.

Compute conditional likelihood under θ in version B: $L^{B,\theta,\alpha}_n = \sum_{j=1}^J g^{\theta}_{n,j} w^{P,\theta}_{n,j} \Big/ \sum_{j=1}^J w^{P,\theta}_{n,j}$.

Compute conditional likelihood under ϕ:$L^{\phi}_n = \frac{1}{J}\sum_{m=1}^J g^{\phi}_{n,m}$.

Select resample indices $k_{1:J}$ with $P(k_j = m) \propto \tilde{g}^{\phi}_{n,m}$.

Obtain resampled particles $X^{F,\theta}_{n,j} = X^{P,\theta}_{n,k_j}$ for $j = 1{:}J$.

Calculate resampled corrected weights:$w^{F,\theta}_{n,j} = w^{P,\theta}_{n,j} \times \frac{g^{\theta}_{n,j}}{g^{\phi}_{n,j}}$ for $j = 1{:}J$.

Compute conditional likelihood under θ in version A: $L^{A,\theta,\alpha}_n = L^{\phi}_n \cdot \sum_{j=1}^J w^{F,\theta}_{n,j} \Big/ \sum_{j=1}^J w^{P,\theta}_{n,j}$.

Return: Likelihood estimate: $\hat{L}(\theta) = \prod_{n=1}^N L^{A,\theta,\alpha}_n$ or $\hat{L}(\theta) = \prod_{n=1}^N L^{B,\theta,\alpha}_n$.

In `pypomp`, DMOP-α is implemented by wrapping the JAX-compiled `mop()` function inside JAX AD. It is a `Pomp` class method calling an internal `_mop_internal()`, which uses static arguments and `jax.lax.fori_loop` for efficiency, and stores weights and likelihoods in log scale to prevent underflow. Systematic sampling is involved for the resampling process. Users can directly apply `jax.grad` and `jax.value_and_grad` to `mop()` to obtain gradients.

In practice, the `mop()` provides an auto-differentiable alternative to `pfilter()`, as a lightweight version. Unlike `pfilter()`, which provides the choice of multiple replicates and diagnostic summaries, `mop()` in `pypomp` focuses purely on producing differentiable likelihood estimates. This makes the algorithm suitable for AD and stochastic gradient descent algorithms in accelerated iterated filtering algorithms by setting the function as input of `jax.value_and_grad()` and `jax.grad()`. Beyond a well-constructed `Pomp` object, the method requires only the number of particles `J`, the evaluation parameter `theta`, a PRNG key, and the cooling factor α. Results are stored in the `results_history` attribute as a list of `jax.Array` objects, one for each parameter set, representing the estimated log-likelihood of the observations. For example, we run

```
LG_obj_3 = pp.Pomp(
```

```
    rinit=rinit,
    rproc=rproc,
    dmeas=dmeas,
    rmeas=rmeas,
    ys=ys,
    theta=theta_list,
    covars=None,
)

LG_obj_3.mop(J = 1000,
             key = subkey,
             alpha = 0.97)
```

Generally, the `result_history` only updates:

- log-likelihood(s): a list of `jax.Array` containing the estimated log-likelihood(s) of the observed data given the model parameters. Always a list, even if only one theta is provided.

This design highlights `mop()` as a lightweight but essential building block for accelarated gradient-based inference methods within `pypomp`. By combining `jax.grad` and `jax.value_and_grad` around `mop()`, the package effectively implements the DMOP algorithm, enabling stochastic-gradient updates for likelihood-based inference on POMP models.

4.3. Iterated Filtering

Iterated filtering (IF2) provides a Monte Carlo approach to estimate parameters by combining particle filtering with sequential random-walk perturbations and cooling. Compared with a plain particle filter or MOP method, IF2 not only evaluates the likelihoods but also systematically updates parameters across iterations. Its primary role is to estimate the parameters that maximizes the likelihood, given the likelihood is intractable but can be estimated under the particle filtering methods. The pseudocode for IF2 algorithm is as follows:

Algorithm 4 Iterated Filtering (IF2)

Require: Starting parameter θ_0; simulator for $f_{X_0}(x_0;\theta)$; simulator for $f_{X_n|X_{n-1}}(x_n \mid x_{n-1};\theta)$; evaluator for $f_{Y_n|X_n}(y_n \mid x_n;\theta)$; data $y^*_{1:N}$; labels $I \subset \{1,\dots,p\}$ for IVPs; fixed lag L; number of particles J; number of iterations M; cooling rate a, $0<a<1$; perturbation scales $\sigma_{1:p}$; initial scale multiplier $C>0$.

for $m = 1$ to M **do**
  Initialize parameters: $\Theta^P_{0,j,i} \sim \text{Normal}\big([\theta_{m-1}]_i,\ (Ca^m\sigma_i)^2\big)$ for $i \in 1{:}p$, $j \in 1{:}J$.
  Initialize states: simulate $X^F_{0,j} \sim f_{X_0}(\cdot;\Theta^P_{0,j})$ for $j = 1{:}J$.
  Initialize filter mean: $\bar\theta_0 = \theta_{m-1}$.
  Define $[V]_i = (C^2+1)a^{2m}\sigma_i^2$.
  for $n = 1$ to N **do**
    Perturb parameters: $\Theta^P_{n,j,i} \sim \text{Normal}\big([\Theta^F_{n-1,j}]_i,\ (a^m\sigma_i)^2\big)$ for $i \notin I$, $j = 1{:}J$.
    Simulate prediction particles: $X^P_{n,j} \sim f_{X_n|X_{n-1}}(\cdot \mid X^F_{n-1,j};\Theta^P_{n,j})$ for $j = 1{:}J$.
    Evaluate weights: $w(n,j) = f_{Y_n|X_n}(y^*_n \mid X^P_{n,j};\Theta^P_{n,j})$ for $j = 1{:}J$.
    Normalize weights: $\tilde w(n,j) = \dfrac{w(n,j)}{\sum_{u=1}^J w(n,u)}$.
    Resample indices $k_{1:J}$ with $\Pr[k_u = j] = \tilde w(n,j)$.
    Resample particles: $X^F_{n,j} = X^P_{n,k_j}$ and $\Theta^F_{n,j} = \Theta^P_{n,k_j}$ for $j = 1{:}J$.
    Filter mean: $[\bar\theta_n]_i = \sum_{j=1}^J \tilde w(n,j)[\Theta^P_{n,j}]_i$ for $i \notin I$.
    Prediction variance: $[V_{n+1}]_i = (a^m\sigma_i)^2 + \sum_{j=1}^J \tilde w(n,j)\left([\Theta^P_{n,j}]_i - [\bar\theta_n]_i\right)^2$ for $i \notin I$.
  end for
  Update non-IVPs: $[\theta_m]_i = [\theta_{m-1}]_i + [V]_i \sum_{n=1}^N \left([\bar\theta_n]_i - [\theta_{m-1}]_i\right)$ for $i \notin I$.
  Update IVPs: $[\theta_m]_i = \frac{1}{J}\sum_{j=1}^J [\Theta^F_{L,j}]_i$ for $i \in I$.
end for

Ensure: Monte Carlo maximum likelihood estimate θ_M.

Under `pypomp`, the IF2 is implemented under `mif()`. Arguments `sigmas` and `sigmas_init` control the random walk standard deviation after and during time t_0 respectively. Another argument `a`, the cooling rate, reduces the perturbation magnitudes across iterations. The purturbations controlled by `sigmas`, `sigmas_init`, and `a` enable the `POMP` model to explore the parameter space and progressively converge to the optimal parameter estimates. Specifically, each call also updates and stores a child key into `LG_obj.fresh_key`, so subfequent method calls can safely omit an explicit assignment on `key` argument.

Different from previous methods for evaluating the likelihoods, `Pomp` methods such as `mif()` can update attributes directly other than `resuts_history`. The `LG_obj.mif()` replaces `LG_obj.theta` with the parameter estimate from the end of the last iteration. The traces of log-likelihoods and parameter estimates are stored in `LG_obj.results_history` as a `xr.DataArray` object. The `xr.DataArray` has dimentions `(replicate, iteration, variable)`, where the `variable` dimension includes the log-likelihood estimations and all POMP model parameters.

:

```
key, subkey = jax.random.split(key)
```

```
#LG_obj_4 = pp.Pomp(
 #   rinit=rinit,
 #   rproc=rproc,
 #   dmeas=dmeas,
 #   rmeas=rmeas,
 #   ys=ys,
 #   theta=theta_list,
 #   covars=None,
#)
#LG_obj_4.mif(
  #sigmas=0.02,
  #sigmas_init=0.1,
  #J=1000,
  #M=100,
  #a=0.5, # cooling rate
  #key=subkey
#)
#LG_obj_4.pfilter(J=1000, reps=36)
#LG_obj_4.mif(
    #sigmas=0.005,
    #sigmas_init=0.0025,
    #J=1000,
    #M=100,
    #a=0.5,
#)
#LG_obj_4.pfilter(J=1000, reps=36)
```

The `pypomp` implementation of IF algorithm in `mif()` inherits the structure of R's `pomp` package while adding JAX compilation, providing a substantial performance improvements over R implementation.

4.4. Iterated Filtering with Automatic Differentiation

Iterated filtering with automatic differentiation (IFAD) (Tan *et al.* 2024) is a hybrid method that combines the complementary advanrages of iterated filtering (IF2) and a new proposed MOP-α gradient method. Here by using the differentiable particle filter, the MOP-α gradient method can obtain gradient and Hessian estimates of the log-likelihood of a POMP model. These estimates are involved in an optimization method to perform a gradient-based search in the parameter space. While IF2 can quickly approach the neighborhood of the global maximum, it struggles to achieve exact local convergence to the global maximum. It can take dozens of iterations to partially close the log-likelihood gap between a point in the neighborhood and the actual global maximum. In contrast, the new MOP-α gradient method can conduct a fast and strong local search, but shows weaker ability at conducting a global exploration (Tan *et al.* 2024). IFAD addresses this tradeoff by first running IF2 to approach the neighborhoold of the global maximum, and then swithcing to the gradient-based method to further refine the parameter estimates. **NOTE:Global Maximum or Local Maximum?**

Algorithm 5 IFAD: Iterated Filtering with Automatic Differentiation

Require: Number of particles J, timesteps N, IF2 cooling schedule η_m, MOP-α discounting parameter α, initial parameter θ_0, iteration index $m = 0$.

1: Run IF2 until initial "convergence" under cooling schedule η_m, or for a fixed number of iterations, to obtain $\{\Theta_j, j = 1, \dots, J\}$.

2: Set $\theta_m := \frac{1}{J}\sum_{j=1}^{J} \Theta_j$.

3: **while** procedure not converged **do**

4: Run Algorithm 3 (MOP-α filter) to obtain $\hat{\ell}(\theta_m)$.

5: Obtain gradient and Hessian:

$$g(\theta_m) = \nabla_{\theta_m}(-\hat{\ell}(\theta_m)), \quad H(\theta_m) \quad \text{s.t. } \lambda_{\min}(H(\theta_m)) > c.$$

6: Update parameter:

$$\theta_{m+1} := \theta_m - \eta_m \, H(\theta_m)^{-1} g(\theta_m).$$

7: Set $m := m + 1$.

8: **end while**

Ensure: Return $\hat{\theta} := \theta_m$.

In `pypomp`, the MOP-α gradent local search is implemented under `train()`, which utilizes JAX's automatic differentiation features with MOP-α to compute the gradient and Hessian of the log-likelihood. While IFAD is not implemented as an independent function, users can always run `mif()` and `train()` to execute the two phases sequentially. For example:

```
key, subkey = jax.random.split(key)
#LG_obj_5 = pp.Pomp(
#    rinit=rinit,
#    rproc=rproc,
#    dmeas=dmeas,
#    rmeas=rmeas,
#    ys=ys,
#    theta=theta_list,
#    covars=None,
#)
#LG_obj_5.mif(
#   sigmas=0.02,
#   sigmas_init=0.1,
# J=1000,
#   M=40,
#   a=0.5,
#   key=subkey
#)
#LG_obj_5.train(
#    J=1000,
#    itns=40,
#    eta=0.0025, # learning rate
#    optimizer="Newton"
```

```
#)
```

Here, `mif()` runs IF2 for 40 iterations, followed by `train()` runs the Newton's method with MOP-α for 40 iterations.

The implemented function `train()` serves as a gradient-based optimizer for exploring the parameter space. Each iteration follows the standard optimization working flow: starting from the current parameter estimate, it computes gradient (and Hessian) of the log-likelihood via `jax.grad()` and `jax.Hessian()`, then utilizes the choosen internal optimizer to update the direction, obtains the learning rate, and finally updates the parameters as well as evaluates the new likelihood under the updated parameters. `train()` supports several common gradient-based optimizers for exploring the parameter space, including Newton's method, weighted Newton's method, Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm, and gradient descent method. In addition, A linear search method (Wills and Schön 2021) is available under `train` for determining the learning rate (step size) under stochastic Quasi-Newton methods.

In `train()`, there is a key argument `n_monitors`, controlling the number of log-likelihood values are evaluated during each training step. When setting `n_monitors=0`, the algorithm totally skip the evaluating process and conduct the gradient-only optimization. It is the fastest choice, but doesn't support the linear search method for learning rate determination, as it utilizes the estimated log-likelihood as the current objective function value. `n_monitors=1` is a lightest monitoring form, where users can get a one log-likelihood evaluation per training step. Larger `n_monitors` reduces the log-likelihood estimate variance in particle filtering using Monte Carlo average at additional computational cost. There is another useful Boolean flag, `scale`, which controls whether the search direction is normalized to unit length. A normalized search direction can provide a more conservative update when the gradients or Hessians are unstable.

Similarly to `mif()`, `train()` updates the `result_history` with the trace of log-likelihoods and parameter estimates as `xr.DataArray` object, and replaces `LG_obj.theta` with the final parameter estimates from the last iteration for each replicate, organized as distionaries keyed by parameter names. The `xr.DataArray` has dimentions `(replicate, iteration, variable)`. The `variable` dimension includes the log-likelihood estimations and all POMP model parameters.

The core highlight of IFAD in algorithmic implementation lies in its internal automatic differentiation and just-in-time compilation powered by JAX. Via JAX, gradients and Hessian matrices for the MOP-α log-likelihood function can be directly obtained without manual derivation, ensuring correctness, efficiency and operability. This also enables flexible use of advanced gradient-based optimizers in each training step, such as Newton's method, quasi-Newton methods, BFGS, gradient descent and stochastic line search. Additionally, JAX's GPU compilation capabilities enable these optimization processes to execute efficiently, making IFAD not only theoretically feasible but also capable of effectively handling large complex POMP models in practical algorithmic implementations.

Data Analysis with pypomp / Tutorials and data analysis examples

This section demonstrates: - Log-likelihood profiling - GPU benchmarking - Conditional log-likelihood residuals

Discussion

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