Adjoint-aided inference of Gaussian process driven differential equations

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airqo
Breathe Clean

GCRF
Global Challenges
Research Fund

EPSRC
Engineering and Physical Sciences
Research Council

Google
Impact Challenge

Outline

- Motivating example: Air pollution in Kampala
- Inference for linear systems:

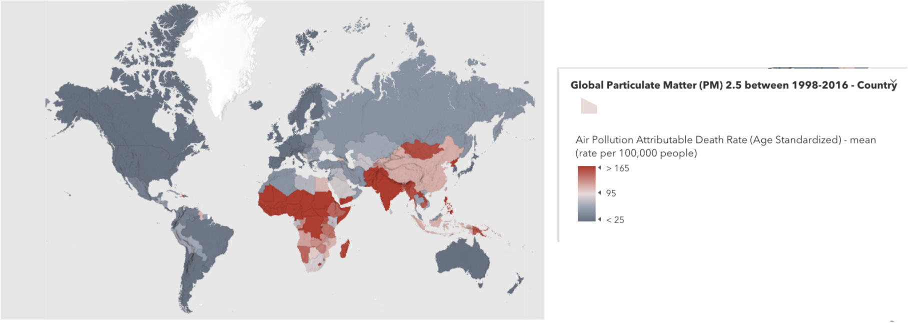
  $$\mathcal{L}u = f$$

  Given noisy measurements of u can we infer f?
- Adjoints

  $$\mathcal{L}^* v \text{ such that } \langle \mathcal{L}u, v \rangle = \langle u, \mathcal{L}^* v \rangle$$
- Examples

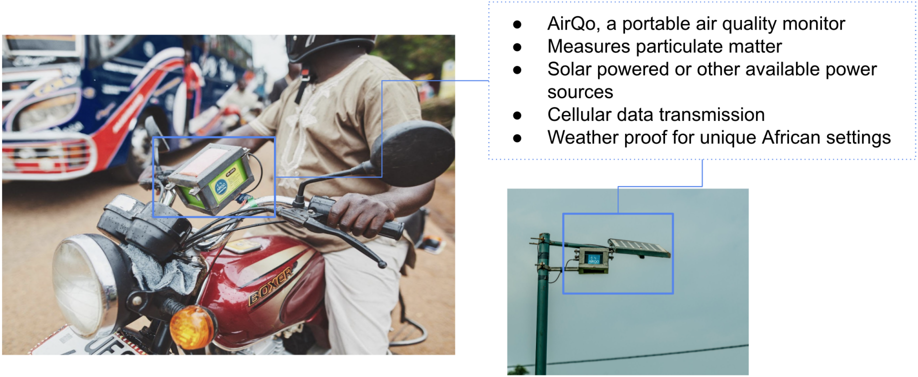
Air pollution

7 million people die every year from exposure to air pollution, the majority in LMICs.


Global Particulate Matter (PM) 2.5 between 1998-2016 - Country
Air Pollution Attributable Death Rate (Age Standardized) - mean (rate per 100,000 people)
> 165
95
< 25

The UK government estimates the annual mortality of human-made air pollution to be 28,000 to 36,000 deaths, and costs UK $\sim$£10^{10}

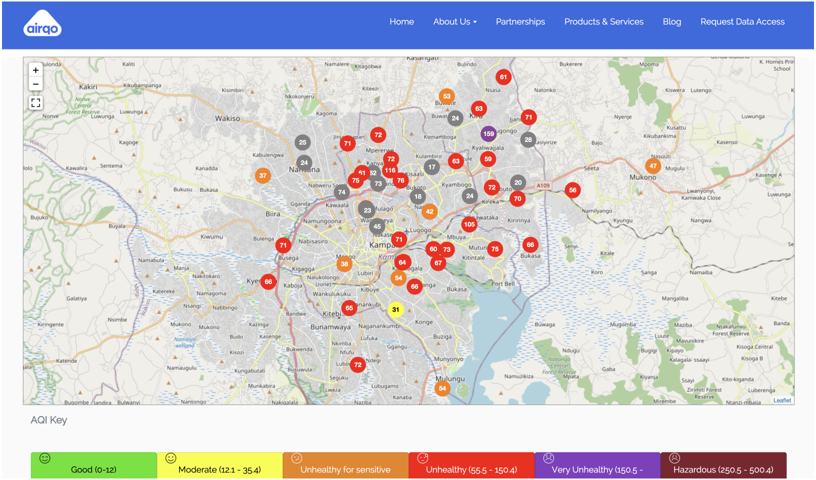
Kampala and AirQo



- AirQo, a portable air quality monitor
- Measures particulate matter
- Solar powered or other available power sources
- Cellular data transmission
- Weather proof for unique African settings

Accurate gravimetric sensors costs $10,000s.
AirQo have developed cheap (but less accurate) sensors that cost $<$ $100 and have deployed them around Kampala.
The sensors measure PM2.5 and PM10.

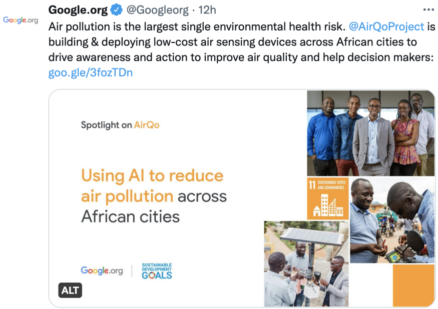
Kampala: PM2.5 levels 12pm yesterday



London (17th of 27 European capitals): 8 $\mu g/m^3$

20 year average for UK: 11 $\mu g/m^3$

WHO guideline: $5\mu g/m^3$



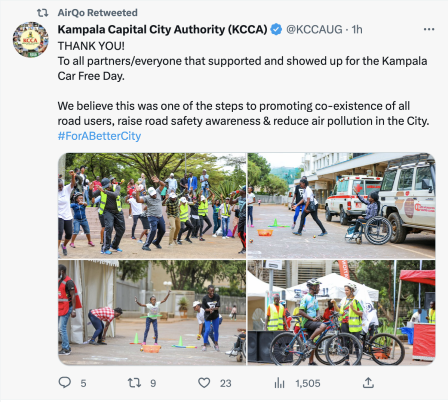
Google.org @Googleorg · 12h

Air pollution is the largest single environmental health risk. @AirQoProject is building & deploying low-cost air sensing devices across African cities to drive awareness and action to improve air quality and help decision makers: goo.gle/3fozTDn

Spotlight on AirQo

Using AI to reduce air pollution across African cities

Google.org | SUSTAINABLE DEVELOPMENT GOALS



AirQo Retweeted

Kampala Capital City Authority (KCCA) @KCCAUG · 1h

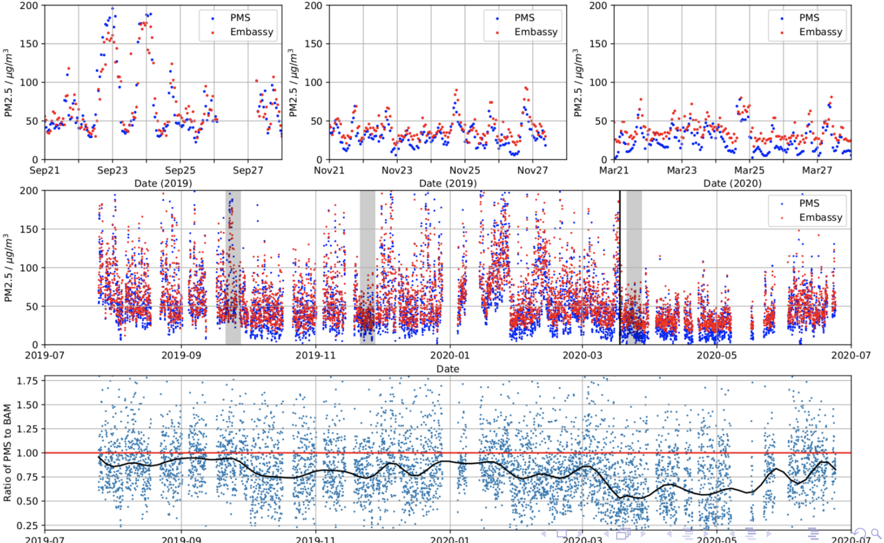
THANK YOU!
To all partners/everyone that supported and showed up for the Kampala Car Free Day.

We believe this was one of the steps to promoting co-existence of all road users, raise road safety awareness & reduce air pollution in the City. #ForABetterCity

Maintaining the calibration of low cost sensors

Smith et al. 2023 JRSS C

- Sensor calibration drifts over time due, e.g., to dust
- Aim to calibrate low cost sensors against 2 reference sensors



Air pollution digital twin

Model pollution concentration $u(x,t)$ at location x time t.
We want to

- infer air pollution (and predict future pollution levels)
- infer pollution sources

Standard non-parametric models (e.g., Gaussian processes) unable to do this.

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Instead build data models that *know* some physics

$$\frac{\partial u}{\partial t} = \nabla.(\mathbf{p}_1 u) + \nabla.(p_2 \nabla u) - p_3 u + \sum_i f_i$$

- $f_i(x, t)$ are different pollution sources,
- we may choose to model different pollution types (PM2.5, PM10 etc)

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Hypothesis: The inclusion of mechanistic behaviour will allow us to infer sources, plan interventions, and predict better.
NB: can also extend the model with a GP to capture missing physics

Computational challenge

Given noisy measurements of pollution levels $z_i = h_i(u) + e_i$.
Can we infer

- the concentration field $u(x, t)$?
- the unknown source terms $f_i(x, t)$?
- the diffusion, advection and reaction parameters? Hyperparameters etc?

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Use Gaussian process priors for $f_i(x, t)$

$$f_i \sim GP(m_i(\cdot), k_i(\cdot, \cdot))$$

where we carefully choose each prior mean and covariance function:

- Industrial regions
- Major roads and power stations
- Varying affluence levels between regions (related to paving of roads, burning of garbage, cooking on solid fuel stoves etc).

General linear systems

$$\mathcal{L}u = f$$

Linear systems with unknown parameters

Consider

$$\mathcal{L}_p u = f$$

where

- $\mathcal{L}_p =$ linear operator with non-linear dependence upon parameters p.
- $f =$ forcing function.
- u is the quantity being modelled, e.g. pollution concentration.

Finding u given p and f is the **forward problem**.

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Inverse problem: infer u, f, p given noisy observations of u

$$z = h(u) + N(0, \Sigma).$$

Note: MCMC likely to be prohibitively expensive: each iteration requires a solution of the forward problem.

Linear systems with unknown parameters

Least squares/maximum-likelihood estimation:

$$\begin{aligned} \min_{p,f} \quad & (z - h(u))^\top (z - h(u)) \\ \text{subject to} \quad & \mathcal{L}_p u = f. \end{aligned}$$

Bayes: find

$$\pi(p, f, u|z).$$

What is an adjoint?

See Estep 2004

Let $\mathcal{L} : \mathcal{U} \to \mathcal{V}$ be a bounded linear operator between Banach spaces, and let $\mathcal{U}^*$ be the dual space of $\mathcal{U}$: the space of bdd linear functionals on $\mathcal{U}$.

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Then F is a bounded linear functional on $\mathcal{U}$, i.e. $F = u^*$ for some $u^* \in \mathcal{U}^*$.

Thus for all $v^* \in \mathcal{V}^*$ we've associated a unique $u^* \in \mathcal{U}^*$.

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By definition

$$v^*(\mathcal{L}(u)) = \mathcal{L}^* v^*(u)$$

which is known as the **bilinear identity**.

Adjoints in Hilbert space

See Estep 2004

When $\mathcal{U}$ and $\mathcal{V}$ are Hilbert spaces

- i.e. vector spaces with an inner product $\langle u, u' \rangle$,

we can identify them with their dual space:

- Riesz representation theorem: for all $v^* \in \mathcal{V}^*$ there exists $v \in \mathcal{V}$ such that $v^* = \langle \cdot, v \rangle_{\mathcal{V}}$

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The **bilinear identity** reduces to

$$\begin{aligned} \langle \mathcal{L}u, v \rangle &= v^*(\mathcal{L}(u)) = \mathcal{L}^* v^*(u) \\ &= \langle u, \mathcal{L}^* v \rangle . \end{aligned}$$

where we now consider $\mathcal{L}^* : \mathcal{V} \to \mathcal{U}$.

Example 0

In the finite dimensional case, $\mathcal{U} = \mathbb{R}^n$, $\mathcal{V} = \mathbb{R}^m$, then $\langle u_1, u_2 \rangle = u_1^\top u_2$ etc and

$$\mathcal{L}u = Au \text{ for some m x n matrix } A.$$

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$$\mathcal{L}u = Au \text{ for some m x n matrix } A.$$

Then

$$\mathcal{L}^* v = A^\top v$$

That is

$$\langle Au, v \rangle = \langle u, A^\top v \rangle$$

Efficient inference

$$\mathcal{L}u = f, \qquad z_i = h_i(u) + e \text{ for } i = 1, \ldots, n$$

If the observation operator is linear

$$h_i(u) = \langle h_i, u \rangle$$

we can consider the n adjoint systems

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Then

$$\begin{aligned} h_i(u) = \langle h_i, u \rangle = \langle \mathcal{L}^* v_i, u \rangle &= \langle v_i, \mathcal{L}u \rangle \\ &= \langle v_i, f \rangle, \end{aligned}$$

by the bilinear identity.

$$z_i = h_i(u) + e_i = \langle v_i, f \rangle + e_i$$
$$\text{where} \quad \mathcal{L}^* v_i = h_i$$

Suppose f is a parametric model with a linear dependence upon some unknown parameters q:

$$f(\cdot) = \sum_{m=1}^{M} q_m \phi_m(\cdot) \tag{1}$$

$$
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$$

A linear model!

The complete observation vector z can then be written as

$$\begin{aligned} z &= \begin{pmatrix} \langle v_1, \phi_1 \rangle & \dots & \langle v_1, \phi_M \rangle \\ \vdots & & \vdots \\ \langle v_n, \phi_1 \rangle & \dots & \langle v_n, \phi_M \rangle \end{pmatrix} \begin{pmatrix} q_1 \\ \\ q_M \end{pmatrix} + e \qquad (2) \\ &= \Phi q + e \end{aligned}$$

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Thus

$$\begin{aligned} \min_{f} \quad & S(f) = (z - h(u))^\top (z - h(u)) \\ \text{subject to} \quad & \mathcal{L}u = f \end{aligned}$$

is equivalent to

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The solution is

$$\hat{q} = (\Phi^\top \Phi)^{-1} \Phi^\top z$$

with $\mathbb{V}\text{ar}(\hat{q}) = \sigma^2 (\Phi^\top \Phi)^{-1}$ when e_i are uncorrelated and homoscedastic with variance σ^2.

In a Bayesian setting, if we assume *a priori* that $q \sim \mathcal{N}_M(\mu_0, \Sigma_0)$, then the posterior for q given z (and other parameters) is

$$q \mid z \sim \mathcal{N}_M(\mu_n, \Sigma_n) \tag{3}$$

where

$$\mu_n = \Sigma_n(\frac{1}{\sigma^2}\Phi^\top z + \Sigma_0^{-1}\mu_0), \quad \Sigma_n = \left(\frac{1}{\sigma^2}\Phi^\top \Phi + \Sigma_0^{-1}\right)^{-1}. \tag{4}$$

Benefits of adjoints

$$\begin{aligned} \min_{p,f} S(p,f) = \quad & (z - h(u))^\top (z - h(u)) \\ \text{subject to} \quad & \mathcal{L}_p u = f. \end{aligned}$$

1. If $f \equiv f_q$ depends linearly on some parameters q we can easily compute the least squares estimator

$$\hat{q}(p) = \arg\min_q S(p, f_q)$$

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This allows for efficient inference of p and f

Quick intro to Gaussian Processes

Suppose we model unknown function $f = \{f(x) : x \in \mathcal{X}\}$ as a Gaussian process (GP)

- i.e. joint distribution of $f(x_1), \ldots, f(x_n)$ is Gaussian.

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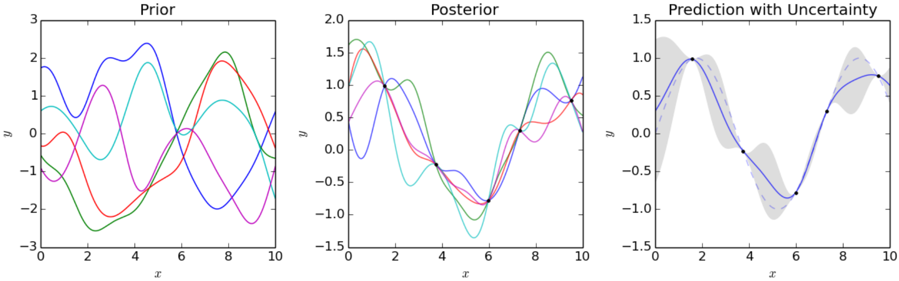
- i.e. joint distribution of $f(x_1), \ldots, f(x_n)$ is Gaussian.

All we need to do is specify the prior mean and covariance functions

$$\mathbb{E}f(x) = m(x), \qquad \mathbb{C}\text{ov}(f(x), f(x')) = k(x, x')$$

$$\text{Write} \qquad f \sim GP(m, k).$$



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- Mathematically attractive family
  - Closed under addition

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    but with updated mean and covariance functions.
  - Closed under any linear operator. If $f \sim GP(m(\cdot), k(\cdot, \cdot))$, then $\mathcal{L}$ is a linear operator

    $$\mathcal{L} \circ f \sim GP(\mathcal{L} \circ m, \mathcal{L}^2 \circ k)$$

    e.g. $\frac{df}{dx}$, $\int f(x)dx$, Af are all GPs

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- Natural - Best linear unbiased predictors etc
- Relate to other methods such as kernel regression

Parameterizing GPs

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- Consider $\{\phi_1(x), \phi_2(x), \ldots\}$ an orthonormal basis for $\mathcal{F}$.

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We can then approximate f using a truncated basis expansion

$$\begin{aligned} f(x) \approx f_q(x) &= \sum_{j=1}^{M} q_i \phi_i(x) \text{ where } \textit{a priori } q_i \sim N(0, \lambda_i^2) \\ &= \Phi \mathbf{q} + e \end{aligned}$$

We've approximated the GP by a linear model.

Choice of basis in $f_q(\cdot) = \sum^M q_i \lambda_i \phi_i(\cdot)$

- **Mercer basis**: $\phi_i(x) = \lambda_i \psi(x)$ where $\lambda_i, \phi_i(\cdot)$ are eigenpairs of

$$T_k(f)(\cdot) = \int_{\mathcal{X}} k(x, \cdot) f(x) \mathrm{d}x.$$

Karhunen-Loève theorem says this choice is mean square optimal

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- **Random Fourier features**: If k stationary, Bochner's theorem:

  $$k(x - x') = \int \exp(iw^\top (x - x'))p(w)dw = \mathbb{E}_{w \sim p} \exp(iw^\top (x - x'))$$

  Thus we can use $\phi_i(x) = \cos(w_i^\top x + b_i)$ where $w_i \sim p(\cdot)$ and $b_i \sim U[0, 2\pi]$

Choice of basis in $f_q(\cdot) = \sum^M q_i \lambda_i \phi_i(\cdot)$

- **Mercer basis**: $\phi_i(x) = \lambda_i \psi(x)$ where $\lambda_i, \phi_i(\cdot)$ are eigenpairs of

  $$T_k(f)(\cdot) = \int_{\mathcal{X}} k(x, \cdot) f(x) \mathrm{d}x.$$

  Karhunen-Loève theorem says this choice is mean square optimal
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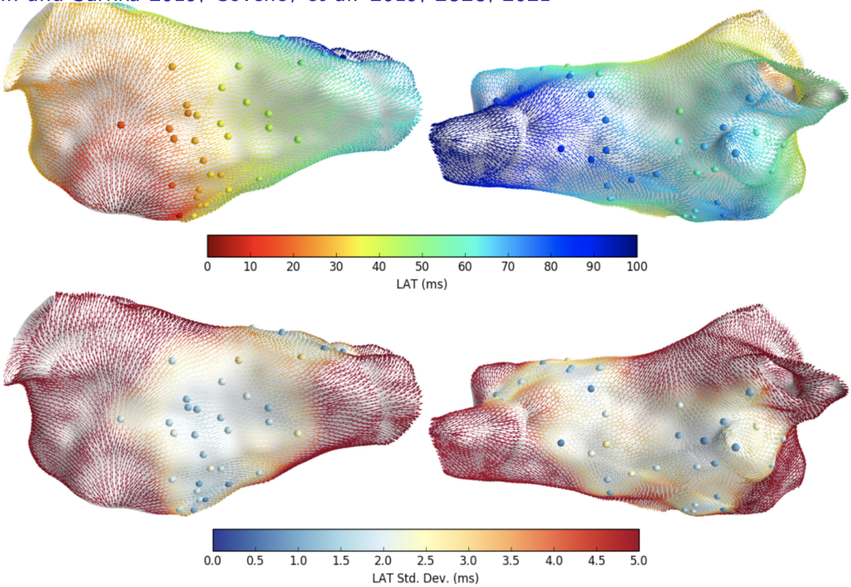
Laplacian basis: useful for non-Euclidean domains

Solin and Sarkka 2019, Coveney et al. 2019, **2020**, 2021



Example 1: Ordinary differential equation

Consider the ordinary differential equation

$$-D\ddot{u} + \nu\dot{u} + u = f(t) \quad \text{with } u(0) = \dot{u}(0) = 0.$$

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$$\begin{aligned}
\langle \mathcal{L}u, v\rangle &= \int_0^T \mathcal{L}u(t)v(t)\mathrm{d}t = \int_0^T (-D\ddot{u} + \nu\dot{u} + u)v\mathrm{d}t \\
&= [-D\dot{u}v]_0^T + \int_0^T D\dot{u}\dot{v}\mathrm{d}t + [\nu uv]_0^T - \int_0^T \nu u\dot{v}dt + \int_0^T uv\mathrm{d}t
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&= [Du\dot{v}]_0^T - \int_0^T Du\ddot{v}\mathrm{d}t - \int_0^T \nu u\dot{v}dt + \int_0^T uv\mathrm{d}t \\
&= \int_0^T (-D\ddot{v} - \nu\dot{v} + v)u\mathrm{d}t \quad \text{when } v(T) = \dot{v}(T) = 0 \\
&= \langle u, \mathcal{L}^* v\rangle
\end{aligned}$$

So the linear operator

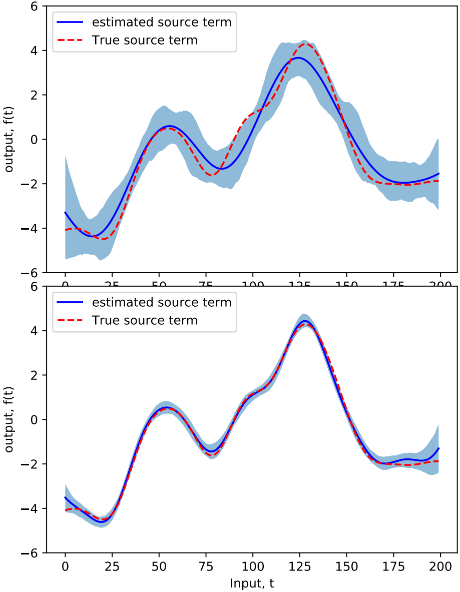
$$\mathcal{L}u = (-D\frac{\mathrm{d}^2}{\mathrm{d}t^2} + \nu\frac{\mathrm{d}}{\mathrm{d}t} + 1)u \quad \text{with } u(0) = \dot{u}(0) = 0$$

has adjoint operator

$$\mathcal{L}^*v = (-D\frac{\mathrm{d}^2}{\mathrm{d}t^2} - \nu\frac{\mathrm{d}}{\mathrm{d}t} + 1)v \quad \text{with } v(T) = \dot{v}(T) = 0$$

The initial conditions for the original system translate to final conditions for the adjoint system.

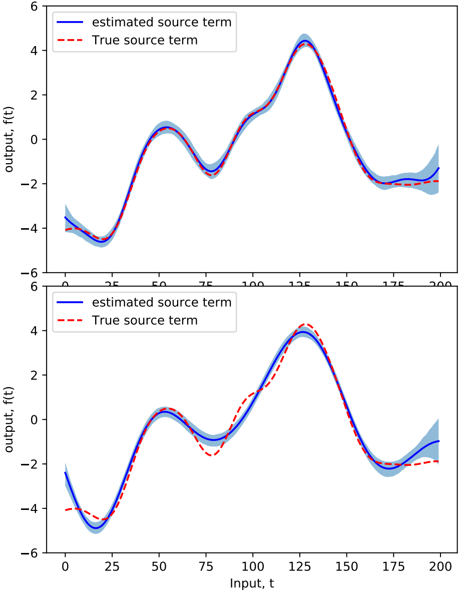
Example 1: Posterior mean and 95% CI (blue), true (red)



- top: $n = 10$ data points, $M = 100$ basis vectors
- bottom: $n = 100$ and $M = 100$

Results required 10 and 100 ODE solves respectively.

Example 1: Too few features



$n = 100$ data points

- top: $M = 100$ basis vectors
- bottom: $M = 10$

NB: overconfident and wrong when $M = 10$ - misspecified model!

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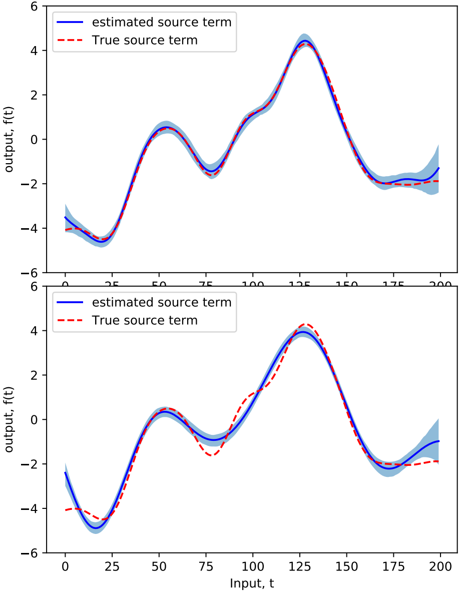

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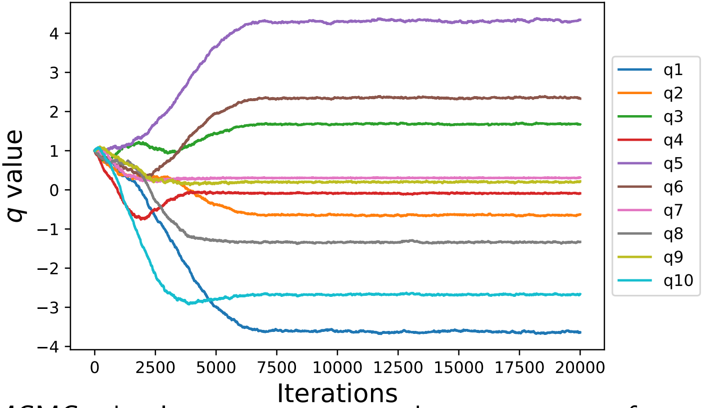
NB: overconfident and wrong when $M = 10$ - misspecified model!

We need enough features to have sufficient modelling flexibility.

Additional features don't require additional ODE solves.

MCMC is fine as long as you have a small number of features.
But even with only 10 features, we need $\sim 1000s$ of ODE solves vs 10 ODE solves for the adjoint method.



MCMC takes longer to converge when we use more features.

Example 2: PDE

Advection-diffusion-reaction is a linear operator:

$$\mathcal{L}u = \frac{\partial u}{\partial t} - \nabla.(\mathbf{p}_1 u) - \nabla.(p_2 \nabla u) + p_3 u$$

Forward problem: solve (for some initial and boundary conditions)

$$\mathcal{L}u = f \text{ on } \mathcal{X} \times [0, T].$$

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h_i are sensor functions that average the pollution at a specific location over a short window

$$\langle h_i, u \rangle = \frac{1}{|\mathcal{T}_i|} \int_{\mathcal{T}_i} u(x_i, t) dt$$

Example 2: PDE adjoint

The adjoint system is again derived by integrating by parts twice:

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$$u(x, 0) = 0 \text{ for } x \in \mathcal{X} \text{ and } \nabla_n u = 0 \text{ for } x \in \partial\mathcal{X}$$

then the final and boundary conditions on the adjoint system are

$$v_i(x, T) = 0 \text{ for } x \in \mathcal{X}$$
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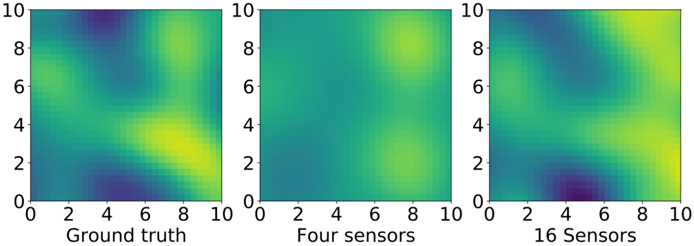
- May find numerical issues: depends on the discretization, the sensor functions h_i, diffusion rate etc
- The cost of solving the adjoint is the same as solving the forward problem.

Results: $n = 20$ (4 sensors) and $n = 80$ (16), noise =10%

Posterior mean of time slice $u(x, 5)$ - more sensors, improved estimates!



Variance of $u(x, 5)$: Wind from the south west.

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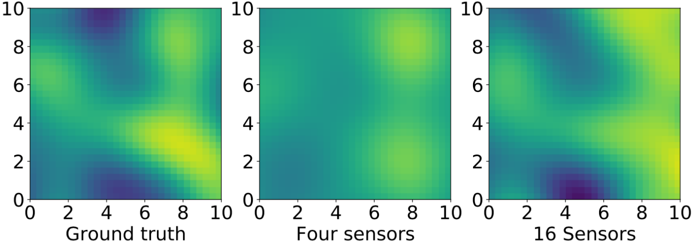
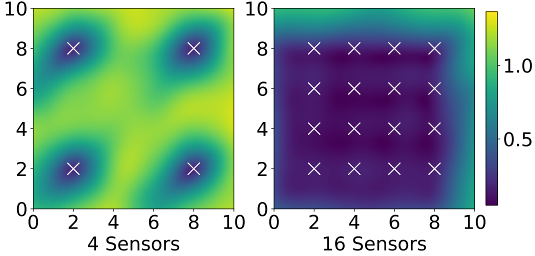


Ground truth

Four sensors

16 Sensors

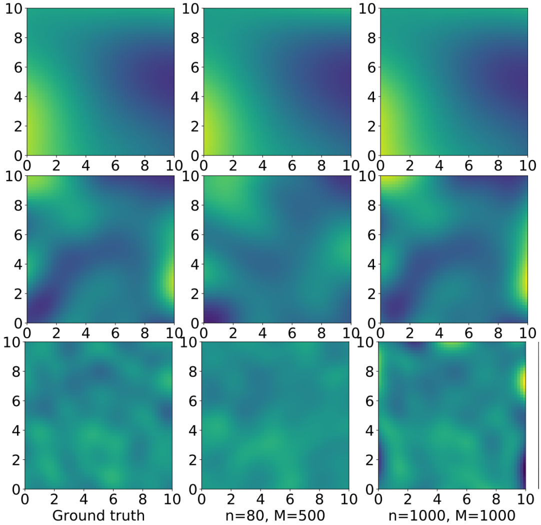
Variance of $u(x, 5)$: Wind from the south west.



4 Sensors

16 Sensors

Effect of length scale, $\lambda = 5, 2, 1$



MSE 0.008 and 0.004

MSE 0.68 and 0.07

MSE 1.85 and 2.55

Example 2: Results

Mean square error vs number of features and sensors

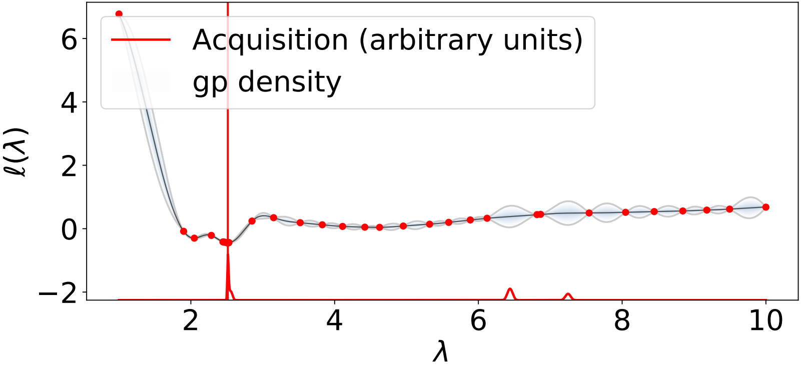
Median MSE as a function of number of sensors and basis vectors.

Sensors			# basis vectors		
	10	50	100	200	300
1	3.42 (2.82,4.39)	3.27 (3.13,3.38)	3.24 (3.10,3.37)	3.27 (3.17,3.44)	3.24
4	7.12 (1.57,28.81)	2.39 (2.06,2.62)	2.41 (2.13,2.60)	2.45 (2.32,2.57)	2.50
9	2.38 (1.41,4.40)	2.12 (1.48,3.98)	1.70 (1.49,2.07)	1.48 (1.40,1.72)	1.47
16	1.73 (1.23,3.28)	3.99 (2.32,10.90)	2.18 (1.72,3.54)	1.3 (1.02,1.68)	1.12
25	1.35 (1.19,3.09)	8.93 (4.92,39.86)	4.36 (2.53,8.20)	1.86 (1.43,2.75)	1.35
25 (MH)	3.27 (1.73,6.12)	-	-	-	-

MH algorithm did not converge after 20,000 iterations for 50 or more RFFs.

Non-linear parameter estimation

A naive way to estimate the non-linear parameters is via Bayesian optimization



- use the adjoint sensitivity to estimate derivative information
- estimate posterior using a variational approach

Sequential data

$$
\begin{aligned}
z &= \begin{pmatrix} \langle v_1, \phi_1 \rangle & \dots & \langle v_1, \phi_M \rangle \\ \vdots & & \vdots \\ \langle v_n, \phi_1 \rangle & \dots & \langle v_n, \phi_M \rangle \end{pmatrix} \begin{pmatrix} q_1 \\ \\ q_M \end{pmatrix} + e \\
&= \Phi \mathbf{q} + e
\end{aligned}
$$

Adding features, or incorporating new data is easy

- New features/basis vectors require new columns in Φ - no new simulation is required
- New data adds rows to Φ - each new data point necessitates one additional simulation.

Costs

Adjoint method:

- require n solves of the adjoint system to infer f.
- (essentially) insensitive to the number of basis functions used.
- The non-linear parameters (GP hyperparameters, PDE parameters) can be inferred in an outer-loop

MCMC:

- All parameters inferred together.
- Hard to say how many iterations will be required, but likely to grow with the the number of parameters (and hence number of GP features).
- Number of iterations required largely independent of n.
- Derivative information generally helps, but may be unavailable (autodiff often unstable for PDE solvers)

Link to Green's function approach

Consider the linear system

$$\mathcal{L}u = f \qquad \text{for } x \in \Omega$$

The Green's function $G_y(x)$ satisfies

$$\mathcal{L}^* G_y(x) = \delta_y(x) \qquad \text{for } x \in \Omega$$

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Solution of the original problem is found by computing the convolution of G with f:

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If $f \sim GP(0, k)$, then u is also distributed as a Gaussian process,

$$u \sim GP(0, k_u)$$

with covariance function

$$k_u(y, y') = \int G_y(x) \int G_{y'}(x') k(x, x') \mathrm{d}x' \mathrm{d}x.$$

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- Expensive, unstable...
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In contrast, adjoint approach relies on

- knowledge of the adjoint operator $\mathcal{L}^*$
- ability to solve adjoint systems numerically - deploy modern finite element solvers (efficient, stable, and offer good error-control).

Recommendation: Use Green's function approach when G is known and covariance integral tractable.

Conclusions

Adjoints are useful

- can be automated
- requires *n* adjoint solves to infer the posterior
  - essentially insensitive to the number of basis functions used
- Gives numerically stable derivatives of the cost function with respect to other parameters, $\frac{\mathrm{d}S}{\mathrm{d}p}$ etc.
- Opportunities for additional efficiencies...
  - Efficient use of adjoint simulations
  - Multi-level approaches
  - Gradient based optimization
  - Sequential data
- Identifiability....
- Enforcing positive forcing
- Extension to system identification...

Ref: Gahungu et al. NeurIPS 2022, Smith et al. 2023 JRSS C.

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Thank you for listening!