Adjoint-aided inference of Gaussian process driven differential equations

Paterne Gahungu[1], Christopher Lanyon[2], Mauricio Alvarez[3],
Engineer Bainomugisha[4], Michael Smith[2]
Richard Wilkinson[5]

[1] Department of Computer Science, University of Burundi
[2] Department of Computer Science, University of Sheffield
[3] Department of Computer Science, University of Manchester
[4] Department of Computer Science, Makerere University
[5] School of Mathematical Sciences, University of Nottingham

September 2022

Project team

Paterne

Engineer

Mike

Mauricio

Chris

Funders:

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:

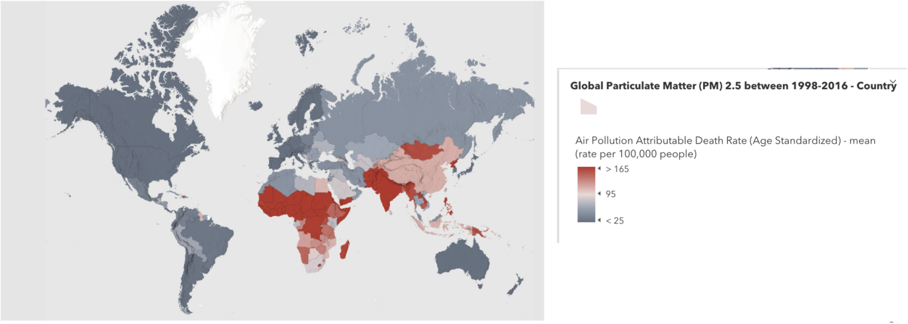
  $$\mathcal{L}u = f$$

  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

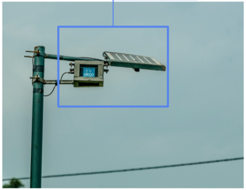
7 million people die every year from exposure to air pollution, the majority in LMICs.


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}

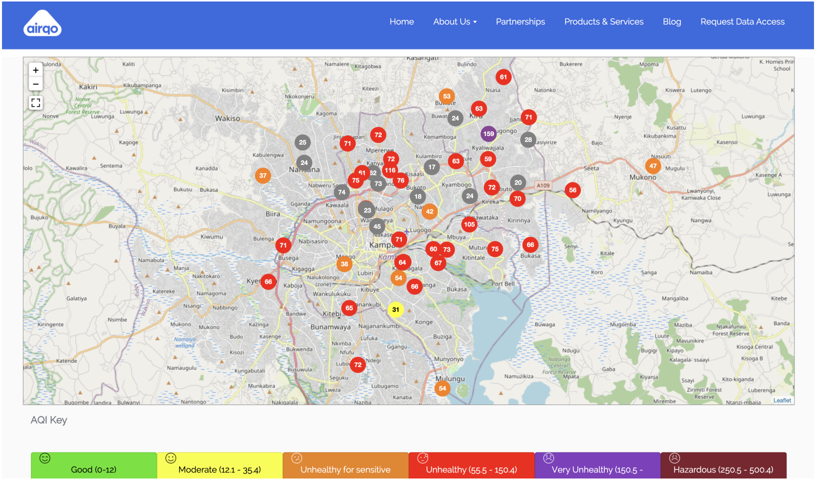
Kampala and AirQo

- 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 at 12pm on 23 Feb 2022

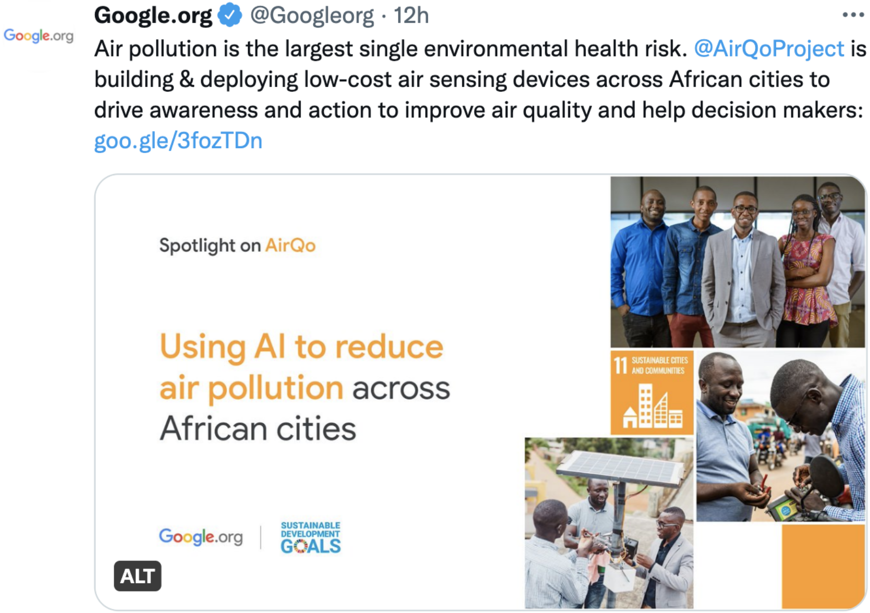


AQI Key

☺ Good (0-12)	☺ Moderate (12.1 - 35.4)	☹ Unhealthy for sensitive	☹ Unhealthy (55.5 - 150.4)	☹ Very Unhealthy (150.5 -	☹ Hazardous (250.5 - 500.4)

Exeter yesterday: 3.1 $\mu g/m^3$

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



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
11 SUSTAINABLE CITIES AND COMMUNITIES
Google.org
SUSTAINABLE DEVELOPMENT GOALS
ALT

Modelling air pollution

Model pollution concentration $u(x, t)$ at location x at 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.

Modelling air pollution

Model pollution concentration $u(x, t)$ at location x at 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.

Instead build data models that *know* some physics

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

Here

- $S_i(x, t)$ are different pollution sources,
- we may choose to model different pollution types (PM2.5, PM10 etc)
- $\mathbf{p}_1$ is related to the wind speed, p_2 is the diffusion tensor, and p_3 the reaction rate.

Modelling air pollution

Model pollution concentration $u(x,t)$ at location x at 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.

Instead build data models that *know* some physics

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

Here

- $S_i(x,t)$ are different pollution sources,
- we may choose to model different pollution types (PM2.5, PM10 etc)
- $\mathbf{p}_1$ is related to the wind speed, p_2 is the diffusion tensor, and p_3 the reaction rate.

Hypothesis: The inclusion of mechanistic behaviour will allow us to infer sources, plan interventions, and predict better.

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 $S_i(x, t)$?
- the diffusion, advection and reaction parameters? Hyperparameters etc?

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 $S_i(x,t)$?
- the diffusion, advection and reaction parameters? Hyperparameters etc?

We will use Gaussian process priors for $S_i(x,t)$

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

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**.

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**.

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

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

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

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

In both cases it would be useful to marginalize parameters, and compute derivatives with respect to the parameters.

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

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

In both cases it would be useful to marginalize parameters, and compute derivatives with respect to the parameters.

- Adjoints can help!

What is an adjoint?

See Estep 2004

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

What is an adjoint?

See Estep 2004

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

Consider $v^* \in \mathcal{V}^*$ and define $F : \mathcal{U} \to \mathbb{R}$ by

$$F : u \mapsto v^*(\mathcal{L}(u)).$$

What is an adjoint?

See Estep 2004

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

Consider $v^* \in \mathcal{V}^*$ and define $F : \mathcal{U} \to \mathbb{R}$ by

$$F : u \mapsto v^*(\mathcal{L}(u)).$$

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 $u^* \in \mathcal{U}^*$.

What is an adjoint?

See Estep 2004

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

Consider $v^* \in \mathcal{V}^*$ and define $F : \mathcal{U} \to \mathbb{R}$ by

$$F : u \mapsto v^*(\mathcal{L}(u)).$$

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 $u^* \in \mathcal{U}^*$.

$$\mathcal{L}^* : v^* \mapsto u^*.$$

$\mathcal{L}^*$ is the **adjoint** of $\mathcal{L}$, and is itself a bounded linear operator.

What is an adjoint?

See Estep 2004

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

Consider $v^* \in \mathcal{V}^*$ and define $F : \mathcal{U} \to \mathbb{R}$ by

$$F : u \mapsto v^*(\mathcal{L}(u)).$$

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 $u^* \in \mathcal{U}^*$.

$$\mathcal{L}^* : v^* \mapsto u^*.$$

$\mathcal{L}^*$ is the **adjoint** of $\mathcal{L}$, and is itself a bounded linear operator.
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 $\langle u, u' \rangle$,

then we can identify them with their dual space:

- by the Riesz representation theorem if $v^* \in \mathcal{V}^*$ there exists $v \in \mathcal{V}$ such that $v^* = \langle \cdot, v \rangle_{\mathcal{V}}$ (and vice versa...).

Adjoints in Hilbert space

See Estep 2004

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

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

then we can identify them with their dual space:

- by the Riesz representation theorem if $v^* \in \mathcal{V}^*$ there exists $v \in \mathcal{V}$ such that $v^* = \langle \cdot, v \rangle_{\mathcal{V}}$ (and vice versa...).

In this case, the **bilinear identity** reduces to

$$\langle \mathcal{L}u, v \rangle_{\mathcal{V}} = v^*(\mathcal{L}(u)) = \mathcal{L}^* v^*(u) = \langle u, \mathcal{L}^* v \rangle_{\mathcal{U}}.$$

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

Adjoints in Hilbert space

See Estep 2004

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

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

then we can identify them with their dual space:

- by the Riesz representation theorem if $v^* \in \mathcal{V}^*$ there exists $v \in \mathcal{V}$ such that $v^* = \langle \cdot, v \rangle_{\mathcal{V}}$ (and vice versa...).

In this case, the **bilinear identity** reduces to

$$\langle \mathcal{L}u, v \rangle_{\mathcal{V}} = v^*(\mathcal{L}(u)) = \mathcal{L}^* v^*(u) = \langle u, \mathcal{L}^* v \rangle_{\mathcal{U}}.$$

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

Example 0: In the finite dimensional case, $\mathcal{L}u = Au$ for some matrix A. Then

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

That is

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

Example 1: Ordinary differential equation

Consider the ordinary differential equation

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

Example 1: Ordinary differential equation

Consider the ordinary differential equation

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

Use the bilinear identity to find the adjoint of

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

Example 1: Ordinary differential equation

Consider the ordinary differential equation

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

Use the bilinear identity to find the adjoint of

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

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

Example 1: Ordinary differential equation

Consider the ordinary differential equation

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

Use the bilinear identity to find the adjoint of

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

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

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

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

Note that initial conditions on the original system translated to final conditions on the adjoint system.

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

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

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

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

- If $z = h(u) + N(0, \Sigma)$, and $q \sim N(m, C)$ a priori, then

$$q \mid z, p = N(m^*, C^*)$$

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

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

    - If $z = h(u) + N(0, \Sigma)$, and $q \sim N(m, C)$ a priori, then

$$q \mid z, p = N(m^*, C^*)$$

2. We can compute $\frac{\mathrm{d}S}{\mathrm{d}p}(p, f_q)$ and approximate $\frac{\mathrm{d}S}{\mathrm{d}p}(p, f_{\hat{q}(p)})$

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

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

   - If $z = h(u) + N(0, \Sigma)$, and $q \sim N(m, C)$ a priori, then

$$q \mid z, p = N(m^*, C^*)$$

2. We can compute $\frac{\mathrm{d}S}{\mathrm{d}p}(p, f_q)$ and approximate $\frac{\mathrm{d}S}{\mathrm{d}p}(p, f_{\hat{q}(p)})$

This may allow for efficient inference of p and f

Efficient inference for q

For our linear system $\mathcal{L}u = f$, suppose

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

When $\mathcal{U}$ and $\mathcal{V}$ are spaces of functions on $\mathcal{X}$, the ϕ_m will also be functions on $\mathcal{X}$. In the finite-dimensional case, the ϕ_m will be vectors of length n.

Efficient inference for q

For our linear system $\mathcal{L}u = f$, suppose

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

When $\mathcal{U}$ and $\mathcal{V}$ are spaces of functions on $\mathcal{X}$, the ϕ_m will also be functions on $\mathcal{X}$. In the finite-dimensional case, the ϕ_m will be vectors of length n. If the observation operator is linear

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

we can consider the n adjoint systems

$$\mathcal{L}_p^* v_i = h_i \text{ for } i = 1, \ldots, n.$$

Efficient inference for q

For our linear system $\mathcal{L}u = f$, suppose

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

When $\mathcal{U}$ and $\mathcal{V}$ are spaces of functions on $\mathcal{X}$, the ϕ_m will also be functions on $\mathcal{X}$. In the finite-dimensional case, the ϕ_m will be vectors of length n. If the observation operator is linear

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

we can consider the n adjoint systems

$$\mathcal{L}_p^* v_i = h_i \text{ for } i = 1, \ldots, n.$$

Then

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

by the bilinear identity.

The i^{th} observation is the inner product between the unknown forcing function f and the solution of the i^{th} adjoint system.

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

The i^{th} observation is the inner product between the unknown forcing function f and the solution of the i^{th} adjoint system.

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

This doesn't appear to have helped.

- To evaluate the likelihood (or sum of squares) we have gone from needing a single forward solve, to n adjoint solves: an n-fold increase in computational cost!

The i^{th} observation is the inner product between the unknown forcing function f and the solution of the i^{th} adjoint system.

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

This doesn't appear to have helped.

- To evaluate the likelihood (or sum of squares) we have gone from needing a single forward solve, to n adjoint solves: an n-fold increase in computational cost!

The benefit arises if there is a linear dependence upon the parameters:

$$h_i(u) = \langle v_i, \sum_{m=1}^{M} q_m \phi_m \rangle = \sum_{m=1}^{M} q_m \langle v_i, \phi_m \rangle.$$

This is a linear model!

The complete observation vector z can then be written as

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

The complete observation vector z can then be written as

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

Thus

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

is equivalent to

$$\min_q \quad S(q) = (z - \Phi q)^\top (z - \Phi q)$$

The complete observation vector z can then be written as

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

Thus

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

is equivalent to

$$\min_q \quad S(q) = (z - \Phi q)^\top (z - \Phi q)$$

The solution is thus

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

with $\mathbb{V}\mathrm{ar}(\hat{q}) = \sigma^2 (\Phi^\top \Phi)^{-1}$ 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

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

Quick intro to Gaussian Processes

Suppose $f = \{f(x) : x \in \mathcal{X}\}$ is an unknown function.

- use a stochastic process to model our uncertainty about f

Quick intro to Gaussian Processes

Suppose $f = \{f(x) : x \in \mathcal{X}\}$ is an unknown function.

- use a stochastic process to model our uncertainty about f

If the joint distribution of $f(x_1), \ldots, f(x_n)$ is Gaussian, we say f is a Gaussian process (GP).

Quick intro to Gaussian Processes

Suppose $f = \{f(x) : x \in \mathcal{X}\}$ is an unknown function.

- use a stochastic process to model our uncertainty about f

If the joint distribution of $f(x_1), \dots, f(x_n)$ is Gaussian, we say f is a Gaussian process (GP).

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

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

We write

$$f \sim GP(m, k).$$

Why use GPs?

- Mathematically attractive
  - Closed under addition

$$f_1, f_2 \sim GP \text{ then } f_1 + f_2 \sim GP$$

Why use GPs?

- Mathematically attractive
  - Closed under addition

$$f_1, f_2 \sim GP \text{ then } f_1 + f_2 \sim GP$$

  - Closed under Bayesian conditioning: if we observe $\mathbf{D} = (f(x_1), \ldots, f(x_n))$ then

$$f|D \sim GP$$

    but with updated mean and covariance functions.

Why use GPs?

- Mathematically attractive
  - Closed under addition

$$f_1, f_2 \sim GP \text{ then } f_1 + f_2 \sim GP$$

  - Closed under Bayesian conditioning: if we observe $\mathbf{D} = (f(x_1), \ldots, f(x_n))$ then

$$f|D \sim GP$$

    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

Why use GPs?

- Mathematically attractive
  - Closed under addition

$$f_1, f_2 \sim GP \text{ then } f_1 + f_2 \sim GP$$

  - Closed under Bayesian conditioning: if we observe $\mathbf{D} = (f(x_1), \ldots, f(x_n))$ then

$$f|D \sim GP$$

    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
- Natural - Best linear unbiased predictors etc

Why use GPs?

- Mathematically attractive
  - Closed under addition

    $$f_1, f_2 \sim GP \text{ then } f_1 + f_2 \sim GP$$

  - Closed under Bayesian conditioning: if we observe $\mathbf{D} = (f(x_1), \ldots, f(x_n))$ then

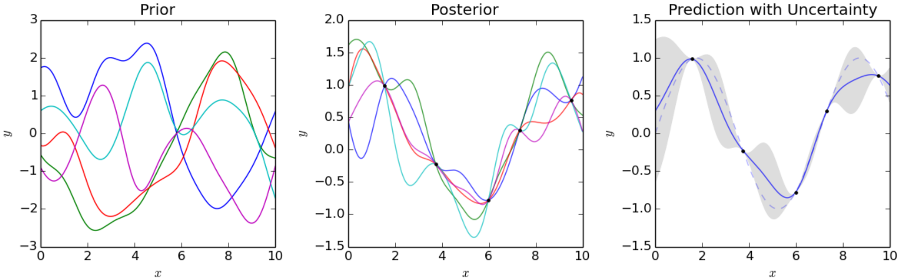
    $$f|D \sim GP$$

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

GP illustration



Parameterizing GPs

$$f(x) \sim GP(m(x), k(x, x')).$$

How can we use GPs within the adjoint framework developed earlier?

Parameterizing GPs

$$f(x) \sim GP(m(x), k(x, x')).$$

How can we use GPs within the adjoint framework developed earlier?

- Let $\mathcal{F}$ be the RKHS (function space) associated with kernel k, i.e., $f \in \mathcal{F}$
- Consider $\{\phi_1(x), \phi_2(x), \ldots\}$ an orthonormal basis for $\mathcal{F}$.

Parameterizing GPs

$$f(x) \sim GP(m(x), k(x, x')).$$

How can we use GPs within the adjoint framework developed earlier?

- Let $\mathcal{F}$ be the RKHS (function space) associated with kernel k, i.e., $f \in \mathcal{F}$
- Consider $\{\phi_1(x), \phi_2(x), \ldots\}$ an orthonormal basis for $\mathcal{F}$.

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 reduced the GP to a linear model.

Choice of basis

- **Mercer basis**: Consider $T_k(f)(\cdot) = \int_{\mathcal{X}} k(x,\cdot)f(x)\mathrm{d}x$. Mercer's theorem gives
$$k(x,x') = \sum_{i=1}^{\infty} \lambda_i \phi_i(x)\phi_i(x')$$
where $\lambda_i, \phi_i(\cdot)$ are eigenpairs of T_k, i.e. $T_k(\phi)(\cdot) = \lambda\phi(\cdot)$
Karhunen-Loève theorem says optimal mean square approximation is
$$\hat{f}(x) = \sum_{i=1}^{M} q_i \sqrt{\lambda_i}\phi_i(x)$$

Choice of basis

- **Mercer basis**: Consider $T_k(f)(\cdot) = \int_{\mathcal{X}} k(x,\cdot) f(x) \mathrm{d}x$. Mercer's theorem gives
$$k(x,x') = \sum_{i=1}^{\infty} \lambda_i \phi_i(x) \phi_i(x')$$
where $\lambda_i, \phi_i(\cdot)$ are eigenpairs of T_k, i.e. $T_k(\phi)(\cdot) = \lambda\phi(\cdot)$
Karhunen-Loève theorem says optimal mean square approximation is
$$\hat{f}(x) = \sum_{i=1}^{M} q_i \sqrt{\lambda_i} \phi_i(x)$$

- **Random Fourier features**: If k stationary, Bochner's theorem:
$$k(x-x') = \int \exp(iw^\top(x-x'))p(w)dw = \mathbb{E}_{w\sim p} \exp(iw^\top(x-x'))$$
$$\approx \frac{1}{M} \sum_{i=1}^{M} (\cos(w_i^\top x), \sin(w_i^\top x)) \begin{pmatrix} \cos(w_i^\top x) \\ \sin(w_i^\top x) \end{pmatrix} \text{ if } w_i \sim p(\cdot)$$
$$\hat{f}(x) = \sum_{i=1}^{M} q_i cos(w_i x + b_i)$$

Example 1: ODE continued

$$-D\ddot{u} + \nu\dot{u} + u = f(t)$$

with $u(0) = \dot{u}(0) = 0$ and $f \sim GP$.
The linear operator and adjoint were

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

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

Example 1: GP expansion

If we write

$$f(t) = \sum_{j=1}^{M} q_j \phi_j(t) = \Phi \mathbf{q}$$

then given observations

$$\begin{aligned} z_i &= \langle h_i, u \rangle + e_i \\ &= \langle v_i, f \rangle + e_i \\ &= v_i^\top \Phi \mathbf{q} + e_i \end{aligned}$$

Example 1: GP expansion

If we write

$$f(t) = \sum_{j=1}^{M} q_j \phi_j(t) = \Phi \mathbf{q}$$

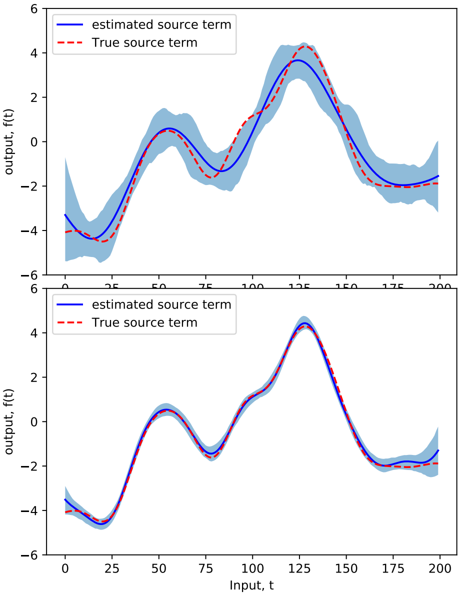
then given observations

$$\begin{aligned} z_i &= \langle h_i, u \rangle + e_i \\ &= \langle v_i, f \rangle + e_i \\ &= v_i^\top \Phi \mathbf{q} + e_i \end{aligned}$$

Thus we can estimate $\mathbf{q}$ by

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

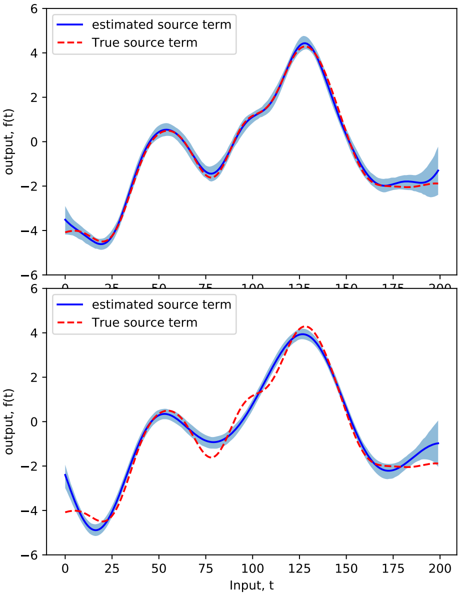
Example 1: Posterior mean and 95% CI (blue), true (red)



- 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

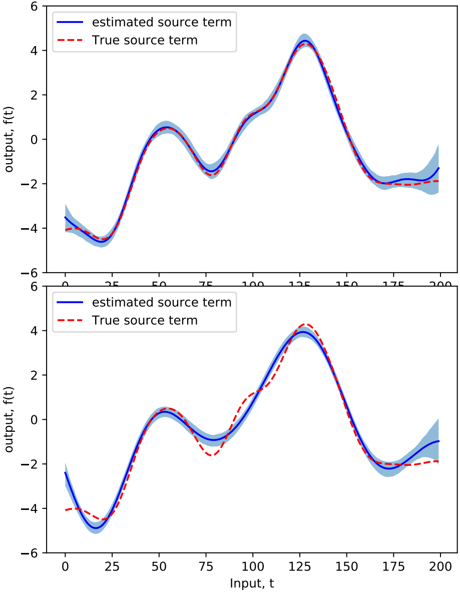


$n = 100$ data points

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

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

Example 1: Too few features



$n = 100$ data points

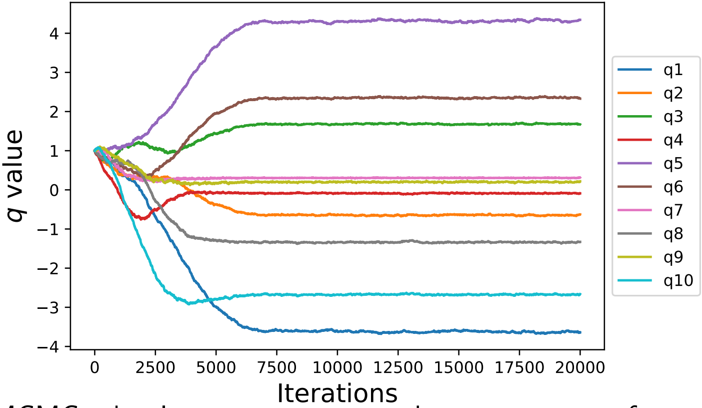
- top: $M = 100$ basis vectors
- bottom: $M = 10$

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

We need to include enough features to have sufficient modelling flexibility.

Using additional features doesn'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:

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

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

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

Example 2: PDE

Advection-diffusion-reaction is a linear operator:

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

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

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

Inverse problem: assume

$$\begin{aligned} f_q(x,t) &\sim GP(m, k_\lambda((x,t),(x',t'))) \\ &\approx \sum_{i=1}^{M} q_i \phi_i(x,t) \text{ where } q_i \sim N(0,1) \end{aligned}$$

and estimate q, p given $z_i = \langle h_i, u \rangle + N(0, \sigma)$.

Example 2: PDE

Advection-diffusion-reaction is a linear operator:

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

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

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

Inverse problem: assume

$$\begin{aligned} f_q(x,t) &\sim GP(m, k_\lambda((x,t),(x',t'))) \\ &\approx \sum_{i=1}^{M} q_i \phi_i(x,t) \text{ where } q_i \sim N(0,1) \end{aligned}$$

and estimate q, p given $z_i = \langle h_i, u \rangle + N(0, \sigma)$.

Typically h_i will be a sensor function that might average the pollution at a specific location over a short window

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

Example 2: PDE adjoint

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

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

Example 2: PDE adjoint

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

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

For n observations we need n adjoint equations!

$$\mathcal{L}^* v_i = h_i \text{ in } \mathcal{X} \times [0, T] \text{ for } i = 1, \ldots, n.$$

Example 2: PDE adjoint

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

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

For n observations we need n adjoint equations!

$$\mathcal{L}^* v_i = h_i \text{ in } \mathcal{X} \times [0, T] \text{ for } i = 1, \ldots, n.$$

If we use initial and boundary conditions

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

then the final and boundary conditions on the adjoint system are

$$v_i(x, T) = 0 \text{ for } x \in \mathcal{X}$$

$$\mathbf{p}_1 v_i(x, t) + p_2 \nabla v_i(x, t) = 0 \text{ for } x \in \partial\Omega \text{ and } t \in [0, T].$$

Example 2: PDE adjoint

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

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

For n observations we need n adjoint equations!

$$\mathcal{L}^* v_i = h_i \text{ in } \mathcal{X} \times [0, T] \;\text{ for } i = 1, \ldots, n.$$

If we use initial and boundary conditions

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

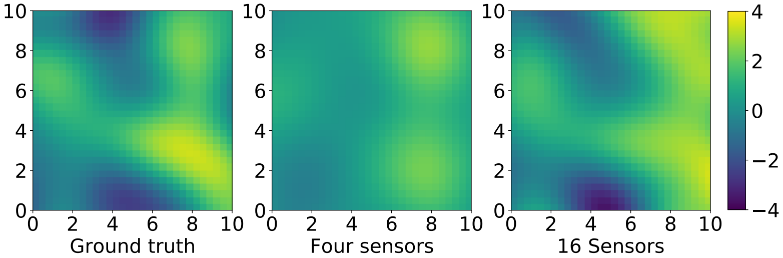
then the final and boundary conditions on the adjoint system are

$$v_i(x, T) = 0 \text{ for } x \in \mathcal{X}$$
$$\mathbf{p}_1 v_i(x, t) + p_2 \nabla v_i(x, t) = 0 \text{ for } x \in \partial\Omega \text{ and } t \in [0, T].$$

- 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%

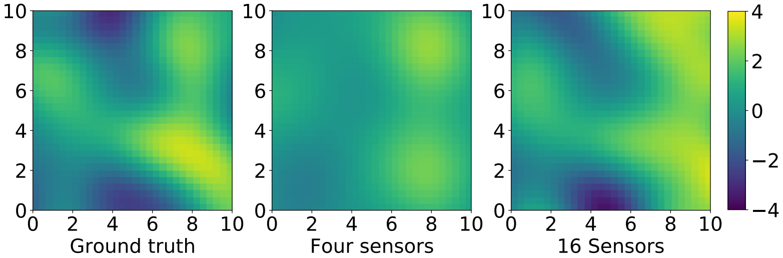
Posterior mean of time slice $u(x, 5)$ - more sensors, improved estimates!



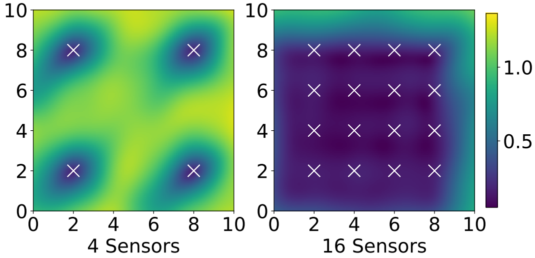
Variance of $u(x, 5)$: Wind from the south west.

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

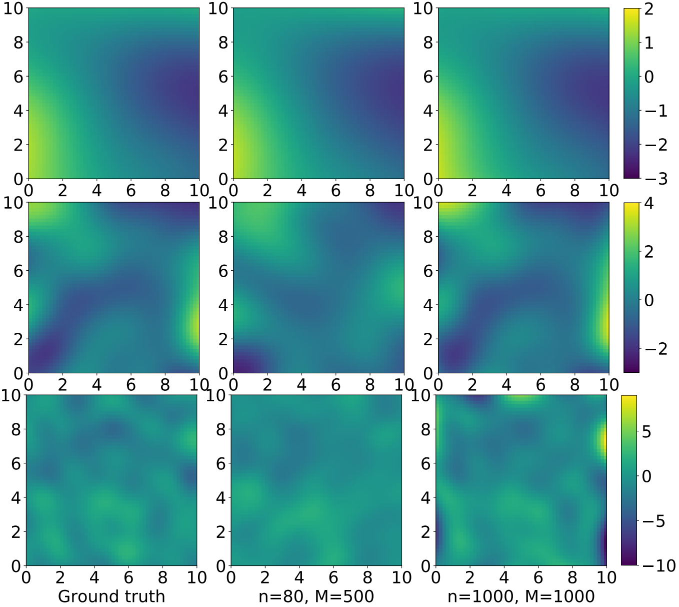
Posterior mean of time slice $u(x, 5)$ - more sensors, improved estimates!



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



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

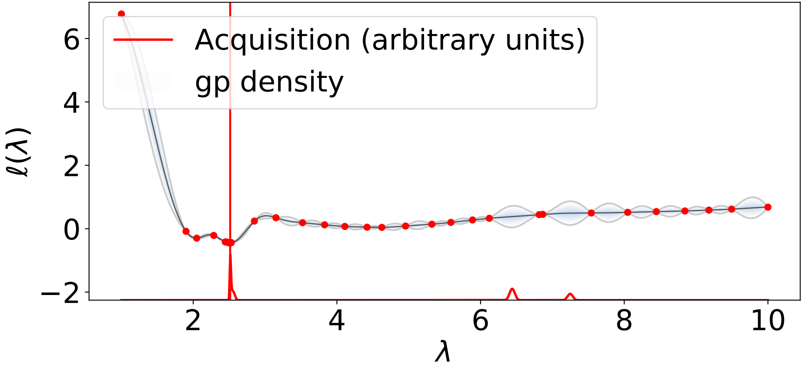
Median MSE as a function of number of sensors and RFFs.

Sensors	Features				
	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 iteration



Preprint showing how to use the adjoint sensitivity soon....

Costs

Adjoint method:

- For the linear forcing/source parameter, we require n solves of the adjoint system to infer the posterior.
- The method is essentially insensitive to the number of basis functions used.
- The non-linear parameters (GP hyperparameters, PDE parameters) can be inferred in an outer-loop - each step requires a further n adjoint solves (and another n forward solves if we want gradient information).

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 this is likely to 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 for this system, $G_y(x)$, satisfies

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

Link to Green's function approach

Consider the linear system

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

The Green's function for this system, $G_y(x)$, satisfies

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

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

$$\begin{aligned} u(y) &= \langle \delta_y, u \rangle = \langle \mathcal{L}^* G_y,\ u \rangle \\ &= \langle G_y,\ \mathcal{L}u \rangle = \langle G_y,\ f \rangle = \int G_y(x) f(x) \mathrm{d}x. \end{aligned}$$

Link to Green's function approach

Consider the linear system

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

The Green's function for this system, $G_y(x)$, satisfies

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

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

$$\begin{aligned} u(y) &= \langle \delta_y, u \rangle = \langle \mathcal{L}^* G_y,\ u \rangle \\ &= \langle G_y,\ \mathcal{L}u \rangle = \langle G_y,\ f \rangle = \int G_y(x) f(x) \mathrm{d}x. \end{aligned}$$

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

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

with covariance function

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

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

If G is known then sometimes it is possible to compute this analytically. Otherwise numerical methods must be used.

- Likely to be cheaper than the adjoint approach

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

If G is known then sometimes it is possible to compute this analytically. Otherwise numerical methods must be used.

- Likely to be cheaper than the adjoint approach

If G is unknown, then need to approximate G before approximating the integral....

- Expensive, unstable...
- Poorly developed

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

If G is known then sometimes it is possible to compute this analytically. Otherwise numerical methods must be used.

- Likely to be cheaper than the adjoint approach

If G is unknown, then need to approximate G before approximating the integral....

- Expensive, unstable...
- Poorly developed

In contrast, our approach relies on

- existence 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 only when G known and covariance integral tractable.

Conclusions

Adjoints of linear systems

- an intrusive method; development does require some work...
- Gives numerically stable derivatives
- For linear parametric forcing models, leads to cheap inference
  - May or may not be faster than MCMC depending on the number of data points, and the dimension of the parameter.

GP models that know some physics can improve predictions over vanilla GPs.

- Lots of opportunities for finding efficiencies...
  - Efficient usage of adjoint simulations
  - Multi-level approaches
  - Gradient based optimization
- See arxiv:2202.04589, to appear NeurIPS 2022.

Conclusions

Adjoints of linear systems

- an intrusive method; development does require some work...
- Gives numerically stable derivatives
- For linear parametric forcing models, leads to cheap inference
  - May or may not be faster than MCMC depending on the number of data points, and the dimension of the parameter.

GP models that know some physics can improve predictions over vanilla GPs.

- Lots of opportunities for finding efficiencies...
  - Efficient usage of adjoint simulations
  - Multi-level approaches
  - Gradient based optimization
- See arxiv:2202.04589, to appear NeurIPS 2022.

Thank you for listening!

Example 1: Matrix system

Suppose $X = Y = \mathbb{R}^d$. A linear operator $\mathcal{L}_p : X \to Y$ can be written as

$$\mathcal{L}_p x = A_p x \text{ where } A_p \in \mathbb{R}^d$$

where A_p depends on unknown parameters p.

The **forward problem** is solving the square linear system $A_p x = f$, i.e., $x_{p,q} = A_p^{-1} f$.

Example 1: Matrix system

Suppose $X = Y = \mathbb{R}^d$. A linear operator $\mathcal{L}_p : X \to Y$ can be written as

$$\mathcal{L}_p x = A_p x \text{ where } A_p \in \mathbb{R}^d$$

where A_p depends on unknown parameters p.

The **forward problem** is solving the square linear system $A_p x = f$, i.e., $x_{p,q} = A_p^{-1} f$.
The **adjoint operator** is

$$\mathcal{L}_p^* y = A_p^\top y$$

as we can see that

$$\begin{aligned} \langle A_p x, y \rangle &= (A_p x)^\top y \\ &= x^\top (A^\top y) \\ &= \langle x, A_p^\top y \rangle \end{aligned}$$

Sensitivity

Consider the quantity of interest (QoI)

$$h(x) \equiv \langle g, x \rangle = g^\top x$$

for some $g \in \mathbb{R}^d$, where x is the solution to $h(x, p) := f - Ax = 0$.

We want to compute $\frac{\mathrm{d}g}{\mathrm{d}p}$ (as then we can compute $\frac{\mathrm{d}S}{\mathrm{d}p}(p, q)$)

Sensitivity

Consider the quantity of interest (QoI)

$$h(x) \equiv \langle g, x \rangle = g^\top x$$

for some $g \in \mathbb{R}^d$, where x is the solution to $h(x,p) := f - Ax = 0$.

We want to compute $\frac{\mathrm{d}g}{\mathrm{d}p}$ (as then we can compute $\frac{\mathrm{d}S}{\mathrm{d}p}(p,q)$)

Define Lagrangian the

$$L = g^\top x + y^\top h(x,p)$$

Think of $y \in \mathbb{R}^d$ as Lagrange multipliers.

$$L = g^\top x + y^\top h(x, p)$$

Differentiating with respect to p gives

$$\frac{dL}{dp} = g^\top \frac{dx}{dp} + y^\top \left(\frac{dh}{dx}\frac{dx}{dp} + \frac{dh}{dp}\right)$$

This is true for all y, so if we set $g^\top + y^\top \frac{dh}{dx} = 0$ then we get

$$\begin{aligned}\frac{dL}{dp} = \frac{dg}{dp} &= y^\top \frac{dh}{dp} \\ &= y^\top \left(\frac{df}{dp} - \frac{dA}{dp}x\right)\end{aligned}$$

where $A^\top y = g$

$$L = g^\top x + y^\top h(x, p)$$

Differentiating with respect to p gives

$$\frac{dL}{dp} = g^\top \frac{dx}{dp} + y^\top\left(\frac{dh}{dx}\frac{dx}{dp} + \frac{dh}{dp}\right)$$

This is true for all y, so if we set $g^\top + y^\top \frac{dh}{dx} = 0$ then we get

$$\begin{aligned}\frac{dL}{dp} = \frac{dg}{dp} &= y^\top \frac{dh}{dp} \\ &= y^\top\left(\frac{df}{dp} - \frac{dA}{dp}x\right)\end{aligned}$$

$$\text{where } A^\top y = g$$

This doesn't require $\frac{\mathrm{d}x}{\mathrm{d}p}$, but does need solutions to the forward $Ax = f$ **and** adjoint systems $A^\top y = g$.

$$L = g^\top x + y^\top h(x, p)$$

Differentiating with respect to p gives

$$\frac{dL}{dp} = g^\top \frac{dx}{dp} + y^\top (\frac{dh}{dx}\frac{dx}{dp} + \frac{dh}{dp})$$

This is true for all y, so if we set $g^\top + y^\top \frac{dh}{dx} = 0$ then we get

$$\begin{aligned} \frac{dL}{dp} = \frac{dg}{dp} &= y^\top \frac{dh}{dp} \\ &= y^\top (\frac{df}{dp} - \frac{dA}{dp} x) \\ \text{where } A^\top y = g \end{aligned}$$

This doesn't require $\frac{\mathrm{d}x}{\mathrm{d}p}$, but does need solutions to the forward $Ax = f$ **and** adjoint systems $A^\top y = g$.

- Autodiff software (eg TensorFlow, JAX etc) will give us this, but can be unreliable for differential equations with long iterative loops

Non-identifiable linear model

Let

$$A_p = \begin{pmatrix} 2+p_2^2 & -1 \\ 1 & 1+p_1^2 \end{pmatrix} \text{ and } f_q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = q_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + q_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and suppose we're given 4 observations with

$$G = \begin{pmatrix} 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{pmatrix}$$

Non-identifiable linear model

Let

$$A_p = \begin{pmatrix} 2 + p_2^2 & -1 \\ 1 & 1 + p_1^2 \end{pmatrix} \text{ and } f_q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = q_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + q_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and suppose we're given 4 observations with

$$G = \begin{pmatrix} 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{pmatrix}$$

Given any dataset we can learn q (given p) with a single adjoint solve.

Non-identifiable linear model

Let

$$A_p = \begin{pmatrix} 2 + p_2^2 & -1 \\ 1 & 1 + p_1^2 \end{pmatrix} \text{ and } f_q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = q_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + q_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and suppose we're given 4 observations with

$$G = \begin{pmatrix} 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{pmatrix}$$

Given any dataset we can learn q (given p) with a single adjoint solve. We can also compute the gradient of $S(p, \hat{q})$ wrt p, but in this case

$$\frac{\mathrm{d}S}{\mathrm{d}p} = 0 \;\forall\; p.$$

and so p is unidentifiable.

Non-identifiable linear model

Let

$$A_p = \begin{pmatrix} 2 + p_2^2 & -1 \\ 1 & 1 + p_1^2 \end{pmatrix} \text{ and } f_q = \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = q_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + q_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

and suppose we're given 4 observations with

$$G = \begin{pmatrix} 2 & 1 & 0 & 1 \\ 1 & 2 & 1 & 0 \end{pmatrix}$$

Given any dataset we can learn q (given p) with a single adjoint solve. We can also compute the gradient of $S(p, \hat{q})$ wrt p, but in this case

$$\frac{\mathrm{d}S}{\mathrm{d}p} = 0 \; \forall \; p.$$

and so p is unidentifiable.

Consider the solution to the unconstrained optimization problem.

$$x^* = \arg\min_x (z - G^\top x)^\top (z - G^\top x)$$

The basis functions used for f form a complete basis for $\mathbb{R}^2$, and we can always find a q so that $A_p x^* = f_q$ (for all p as A_p is invertible).