UQ of Model Discrepancy using Gaussian Processes

with applications to sound field control

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Sound field control part is joint work with:

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The core issue: Approximating model discrepancies

Consider the physical system

$$y = \mathcal{P}(x) + e,$$

where $\mathcal{P}$ is a physical “forward” operator, x the input, y the measured output and e measurement noise.

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- $\mathcal{M}(x, \theta)$ will depend on model parameters θ. We need to estimate these.
- We are interested in approximating $\mathcal{P}(x)$ as accurately as possible. (It may later be used for inference, extrapolation etc.)
- It is the case that $\mathcal{M}$ is a simplification of $\mathcal{P}$ and thus there are some phenomena that $\mathcal{M}$ does not capture. Can we take this model discrepancy into account?

The core issue: Approximating model discrepancies

The typical model approximation:

$$\begin{aligned} y &= \mathcal{P}(x) + e \\ &\approx \mathcal{M}(x, \theta) + e \end{aligned}$$

The model discrepancy approximation:

$$\begin{aligned} y &= \mathcal{P}(x) + e \\ &= \mathcal{M}(x, \theta) + (\mathcal{P}(x) - \mathcal{M}(x, \theta)) + e \\ &\approx \mathcal{M}(x, \theta) + \delta_\beta(x) + e \end{aligned}$$

where (in this talk) $\delta_\beta(x)$ is a Gaussian Process (more on those soon).

References on model discrepancy: [Kennedy 2001], [Brynjarsdóttir 2014], ...

What can it do?

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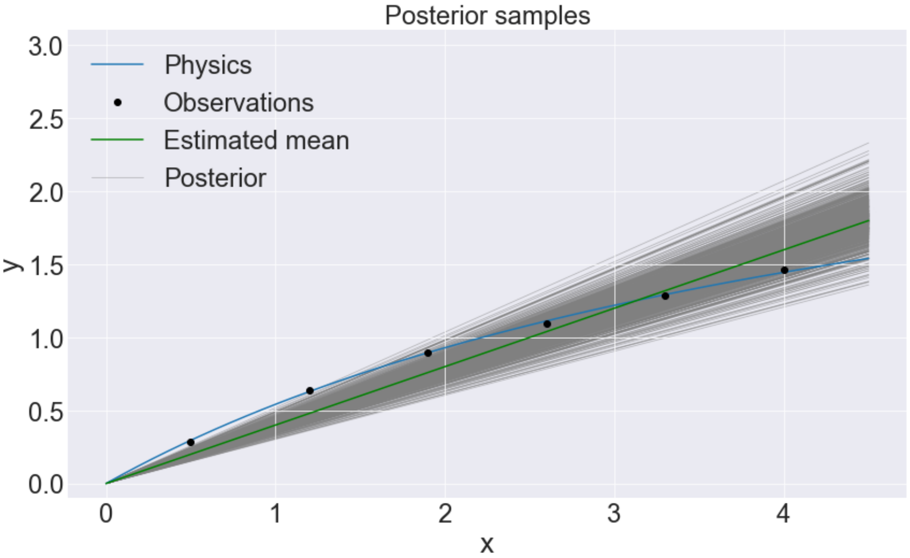
Improved accuracy of model and tighter uncertainty bounds.

Using model: $y = \mathcal{M}(x, \theta) + e$



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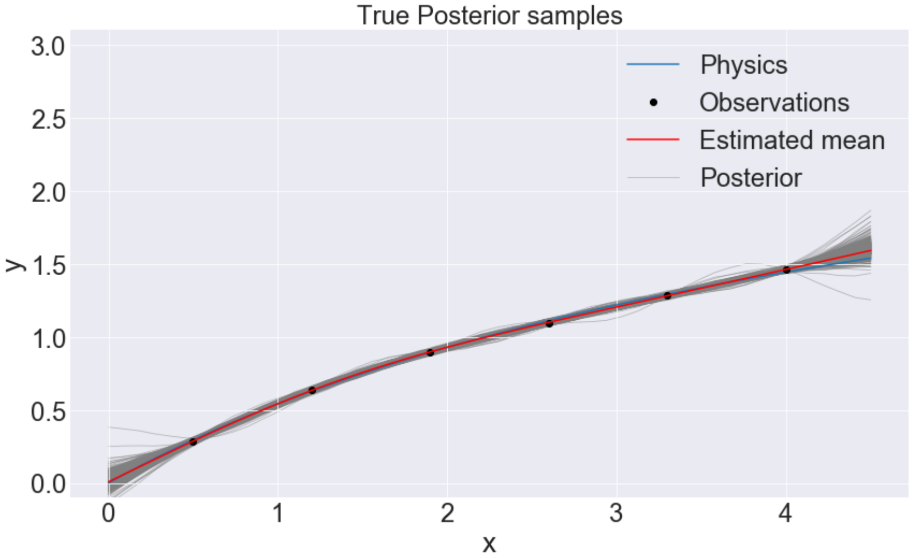
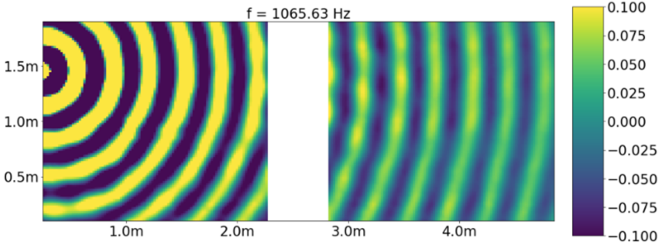
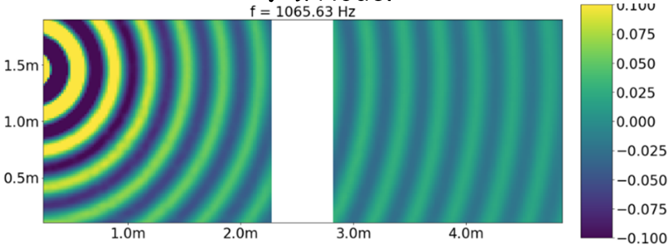


What can it do?

$\mathcal{P}$: Actual transfer function



$\mathcal{M}$: Model



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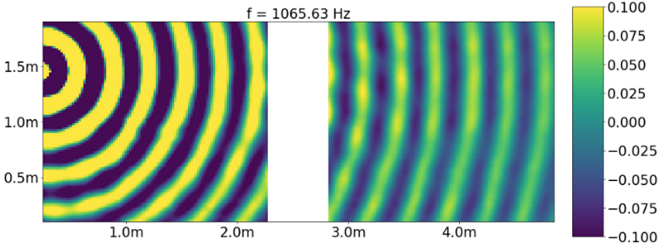
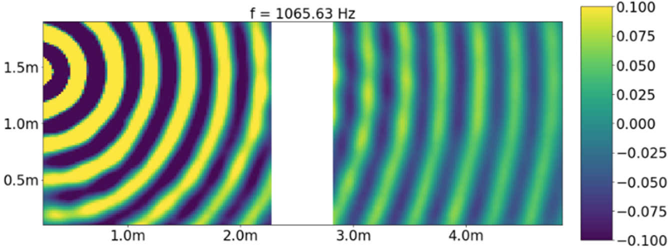


$\mathcal{M} + \delta_\beta$: Model + Gaussian Process



What does it need?

The model discrepancy approximates

$$\delta_\beta(x) \approx \mathcal{P}(x) - \mathcal{M}(x, \theta).$$

Typically we need either one of the following.

- Strong prior on model discrepancy.
- Enough observations of $\mathcal{P}(x) + e$.

Outline

- Theory: Gaussian Processes
- Theory: Bayesian inversion / parameter estimation
- Application: Toy example
- Application: Sound field control for outdoor concerts

Theory: Gaussian Processes

Gaussian Processes

A Gaussian Process (GP) is completely specified by its mean and covariance function. For a process $\delta(x)$ we define the mean and covariance as

$$m(x) = \mathbb{E}[\delta(x)]$$
$$k(x, x') = \mathbb{E}[(\delta(x) - m(x))(\delta(x') - m(x'))]$$

and write the GP as

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Example: The zero mean and squared exponential GP:

$$m(x) = 0$$
$$k_{s,l}(x,x') = s^2 \exp\left(-\frac{\|x - x'\|^2}{2l^2}\right)$$

Gaussian Processes as prior distribution

For a fixed grid, $\mathbf{x} \in \mathbb{R}^m$, the GP defines a normal distribution, i.e,

$$\mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x})) = \mathcal{N}(\boldsymbol{\mu}, \mathbf{K}),$$

where $\boldsymbol{\mu} = m(\mathbf{x}) \in \mathbb{R}^m$ and $\mathbf{K} = k(\mathbf{x}, \mathbf{x}) \in \mathbb{R}^{m \times m}$.

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Thus if we use the GP as a prior on $\delta(x)$, we may define the vector

$$\boldsymbol{\delta}_\mathbf{x} \sim \mathcal{GP}(m(\mathbf{x}), k(\mathbf{x}, \mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \mathbf{K}).$$

We can then estimate (from measured data) $\boldsymbol{\delta}_\mathbf{x}$, and then determine $\delta(x)$ on another domain $\mathbf{x}^*$ by conditioning on $\mathbf{x}^*, \mathbf{x}, \boldsymbol{\delta}_\mathbf{x}$.

Gaussian Process conditioning

If $\delta(x)$ follows a GP, we may define two vectors $\boldsymbol{\delta}_{\mathbf{x}}$ and $\boldsymbol{\delta}_{\mathbf{x}^*}$ from the GP, which will follow a joint normal:

$$\begin{bmatrix} \boldsymbol{\delta}_{\mathbf{x}} \\ \boldsymbol{\delta}_{\mathbf{x}^*} \end{bmatrix} \sim \mathcal{N}\left(0, \begin{bmatrix} k(\mathbf{x},\mathbf{x}) & k(\mathbf{x},\mathbf{x}^*) \\ k(\mathbf{x}^*,\mathbf{x}) & k(\mathbf{x}^*,\mathbf{x}^*) \end{bmatrix}\right)$$

Then using results of joint normal distributions, we may condition on $\mathbf{x}$, $\boldsymbol{\delta}_{\mathbf{x}}$ and $\mathbf{x}^*$ to get $\boldsymbol{\delta}_{\mathbf{x}^*}$ as follows.

$$\begin{aligned} &\boldsymbol{\delta}_{\mathbf{x}^*} | \mathbf{x}^*, \mathbf{x}, \boldsymbol{\delta}_{\mathbf{x}} \\ &\sim \mathcal{N}\left(k(\mathbf{x}^*,\mathbf{x})k(\mathbf{x},\mathbf{x})^{-1}\boldsymbol{\delta}_{\mathbf{x}},\ k(\mathbf{x}^*,\mathbf{x}^*) - k(\mathbf{x}^*,\mathbf{x})k(\mathbf{x},\mathbf{x})^{-1}k(\mathbf{x},\mathbf{x}^*)\right) \end{aligned}$$

For more details see, e.g., [Rasmussen 2006].

Summary of model discrepancy approach

Consider the problem of determining the following model from observations

$$\mathbf{y} = \mathcal{M}(\mathbf{x}, \boldsymbol{\theta}) + \boldsymbol{\delta}_{\mathbf{x}} + \mathbf{e},$$

where $\mathbf{e} \sim \mathcal{N}(0, \sigma^2 \mathbf{I})$, $\boldsymbol{\theta} \sim \pi(\boldsymbol{\theta})$ and $\boldsymbol{\delta}_{\mathbf{x}} = \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x})) = \mathcal{N}(0, \mathbf{K})$.
First estimate $[\boldsymbol{\theta}; \boldsymbol{\delta}_x] \in \mathbb{R}^{p+m}$ from observations. Then define the model:

$$\mathcal{M}(\mathbf{x}^*, \boldsymbol{\theta}) + \boldsymbol{\delta}_{\mathbf{x}^*} \,|\, \mathbf{x}^*, \mathbf{x}, \boldsymbol{\delta}_{\mathbf{x}}.$$

The conditional mean is given by

$$\mathbf{y}^*_{\text{cm}}(\boldsymbol{\theta}) = \mathcal{M}(\mathbf{x}^*, \boldsymbol{\theta}) + k(\mathbf{x}^*, \mathbf{x}) k(\mathbf{x}, \mathbf{x})^{-1} \boldsymbol{\delta}_{\mathbf{x}}.$$

The full distribution is given by

$$\mathcal{N}(\mathbf{y}^*_{\text{cm}}(\boldsymbol{\theta}), K_{\mathbf{x}^*\mathbf{x}}),$$

where $K_{\mathbf{x}^*\mathbf{x}} = k(\mathbf{x}^*, \mathbf{x}^*) - k(\mathbf{x}^*, \mathbf{x}) k(\mathbf{x}, \mathbf{x})^{-1} k(\mathbf{x}, \mathbf{x}^*)$.

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Theory: Bayesian inversion / parameter estimation

Standard model approximation

Given model

$$y = \mathcal{M}(x,\theta) + e, \quad e \sim \mathcal{N}(0,\sigma^2 I),\ \theta \sim \pi(\theta).$$

Bayes rule yields:

$$\pi(\theta|y) \propto \pi(y|\theta)\pi(\theta),$$

where the likelihood is

$$\pi(y|\theta) \propto \exp\left(-\frac{1}{2\sigma^2}\|y-\mathcal{M}(x,\theta)\|_2^2\right),$$

and hence posterior is given by

$$\pi(\theta|y) \propto \exp\left(-\frac{1}{2\sigma^2}\|y-\mathcal{M}(x,\theta)\|_2^2\right)\pi(\theta).$$

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Including hyper parameters

$$\pi(\theta,\alpha,\sigma|y) \propto \exp\left(-\frac{1}{2\sigma^2}\|y - \mathcal{M}(x,\theta)\|_2^2\right)\pi(\theta|\alpha)\pi(\alpha)\pi(\sigma).$$

For more details see, e.g., [Bardsley 2018], ...

Model discrepancy approximation

Given model

$$y = \mathcal{M}(x,\theta) + \delta_x + e, \quad e \sim \mathcal{N}(0,\sigma^2 I),\ \theta \sim \pi(\theta),\ \delta_x \sim \mathcal{N}(0,K_x)$$

Assuming δ_x independent of θ (!) Bayes rule yields:

$$\pi(\theta,\delta_x|y) \propto \pi(y|\theta,\delta_x)\pi(\theta)\pi(\delta_x),$$

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Hyper parameters

$$\pi(\theta, \alpha, \beta, \sigma | y)$$
$$\propto \exp\left(-\frac{1}{2\sigma^2}\|y - \mathcal{M}(x, \theta) - \delta_x\|_2^2\right)\pi(\theta|\alpha)\pi(\alpha)\pi(\delta_x|\beta)\pi(\beta)\pi(\sigma)$$

Model discrepancy: The linear Gaussian case

Suppose $\boldsymbol{\theta} \sim \mathcal{N}(\boldsymbol{\theta}_0, \mathbf{K}_{\boldsymbol{\theta}})$ and that the model is linear, i.e., $\mathcal{M}(\mathbf{x}, \boldsymbol{\theta}) = \mathbf{A}\boldsymbol{\theta}$. Then we have the posterior

$$\pi(\boldsymbol{\theta}|\mathbf{y}) \propto \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{y} - \mathbf{G}\mathbf{u}\|_2^2 - \frac{1}{2}\mathbf{u}^T\mathbf{K}^{-1}\mathbf{u}\right)$$
$$\propto \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{y} - \mathbf{G}\mathbf{u}\|_2^2 - \frac{1}{2}\|\mathbf{L}\mathbf{u}\|_2^2\right),$$

with MAP estimate

$$\mathbf{u}_{\text{map}} = \frac{1}{\sigma^2}\|\mathbf{y} - \mathbf{G}\mathbf{u}\|_2^2 + \|\mathbf{L}\mathbf{u}\|_2^2,$$

where

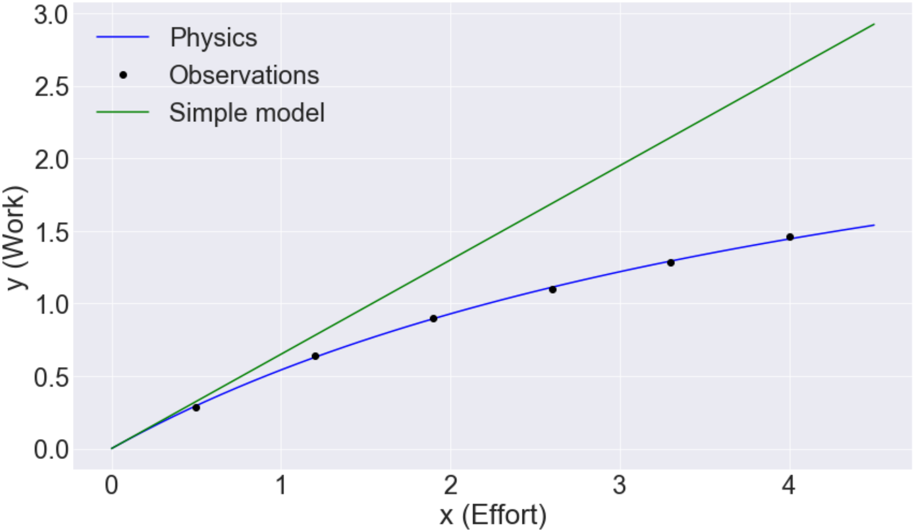
$$\mathbf{G} = \begin{bmatrix}\mathbf{A} & \mathbf{I}\end{bmatrix}, \quad \mathbf{u} = \begin{bmatrix}\boldsymbol{\theta} \\ \boldsymbol{\delta}_{\mathbf{x}}\end{bmatrix} \sim \mathcal{N}(\mathbf{0}, \mathbf{K}),$$

$\mathbf{K} = \begin{bmatrix}\mathbf{K}_{\boldsymbol{\theta}} & 0 \\ 0 & \mathbf{K}_{\mathbf{x}}\end{bmatrix}$ and $\mathbf{L}^T\mathbf{L} = \mathbf{K}$.

Application: Toy example

Toy example set-up

$$\mathcal{P}(x) = \frac{0.65x}{1 + x/5}, \; \mathcal{M}(x, \theta) = \theta x.$$



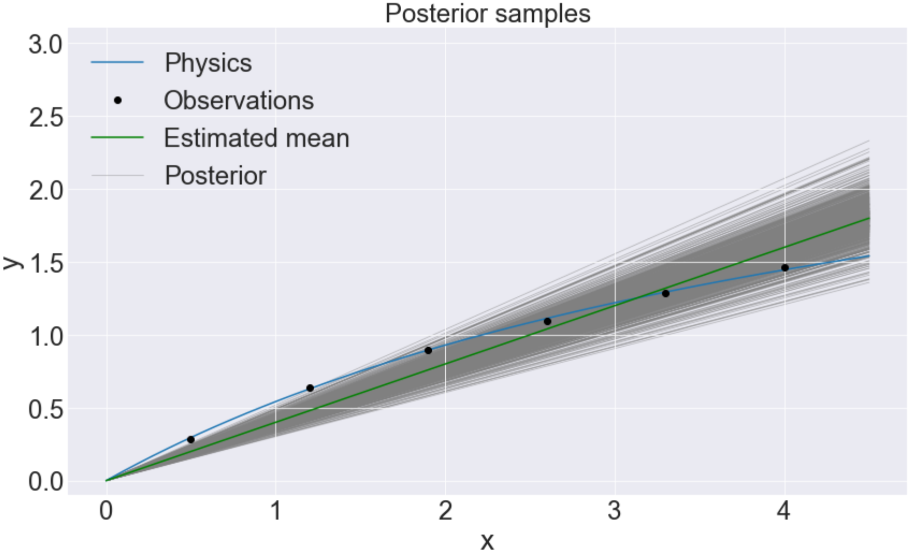
Standard approximation with MCMC solver: PyMC code

https://github.com/pymc-devs/pymc3

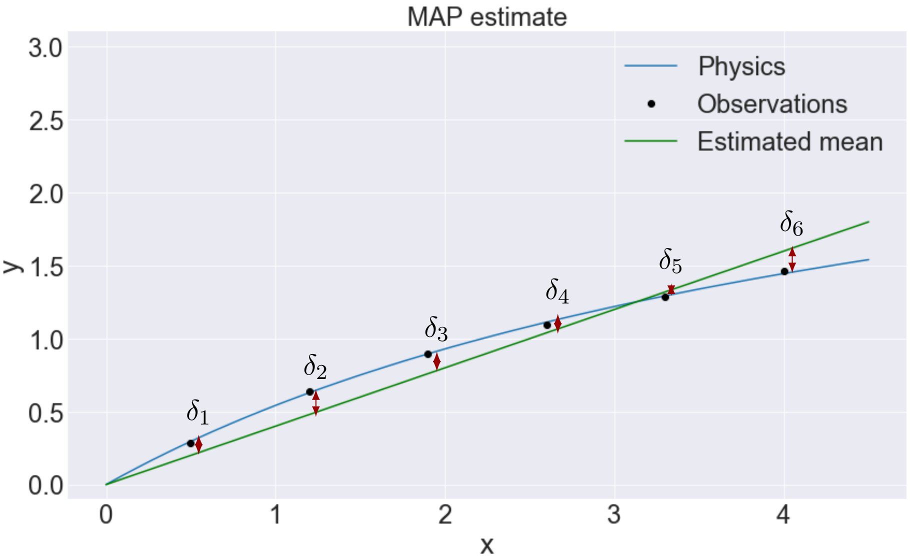
```
#hyper priors
sigma = pm.Gamma('sigma',alpha=1,beta=1e-4)
eta   = pm.Gamma('eta',alpha=1,beta=1e-4)

#Prior
theta = pm.Normal('theta',mu=0,sd=eta)

#Expected value of outcome
mu = theta*x

#Likelihood
y = pm.Normal('y', mu=mu, sd=sigma, observed=d)
```

Standard approximation with MCMC solver: solution

Using model: $y = \mathcal{M}(x, \theta) + e$



How much δ is needed to better fit the measurements?



Including Gaussian Process

```
#Hyper priors
sigma = pm.Gamma('sigma',alpha=1,beta=1e-4)
eta   = pm.Gamma('eta',alpha=1,beta=1e-4)
s     = pm.HalfNormal('s',sd=1)
l     = pm.HalfNormal('l',sd=1)

#Define GP
gp    = pm.gp.Latent(cov_func=(s**2)*pm.gp.cov.ExpQuad(1,l))

#Priors
theta = pm.Normal('theta',mu=0,sd=eta)
delta = gp.prior('delta',X=x[:,None])

#Expected value of outcome
mu = theta*x+delta

#Likelihood
y = pm.Normal('y', mu=mu, sd=sigma, observed=d)
```

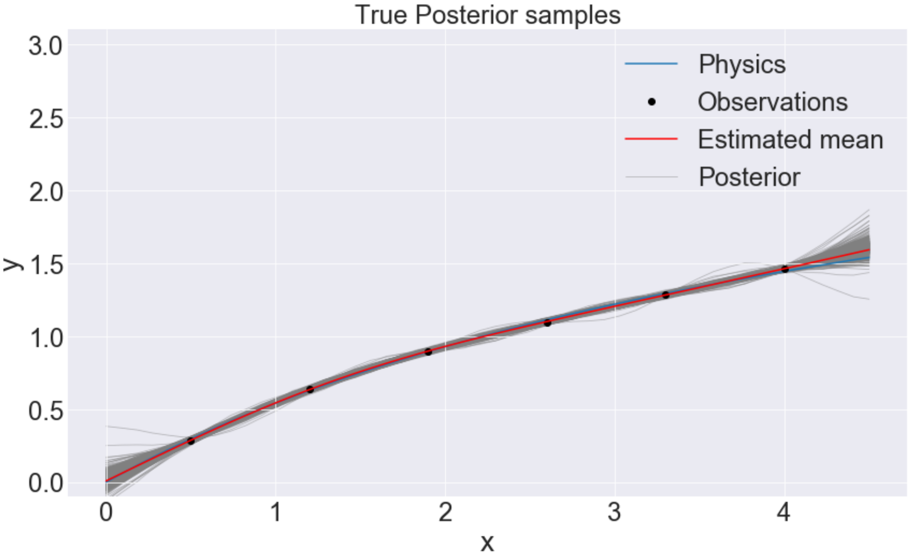
Model discrepancy approximation with MCMC solver: PyMC code

Recall that once $\boldsymbol{\delta}_{\mathbf{x}}$ is estimated, we can sample $\boldsymbol{\delta}_{\mathbf{x}^*}$ on a new grid $\mathbf{x}^*$ since

$$\begin{aligned}&\boldsymbol{\delta}_{\mathbf{x}^*}|\mathbf{x}^*, \mathbf{x}, \boldsymbol{\delta}_{\mathbf{x}}\\ &\sim \mathcal{N}\left(k(\mathbf{x}^*,\mathbf{x})k(\mathbf{x},\mathbf{x})^{-1}\boldsymbol{\delta}_{\mathbf{x}},\; k(\mathbf{x}^*,\mathbf{x}^*) - k(\mathbf{x}^*,\mathbf{x})k(\mathbf{x},\mathbf{x})^{-1}k(\mathbf{x},\mathbf{x}^*)\right)\end{aligned}$$

Including Gaussian Process

Using model: $y = \mathcal{M}(x, \theta) + \delta_\beta(x) + e$



Application: Sound field control for outdoor concerts

Why do we need to control sound at outdoor concerts?

Concerts in cities cause nearby residents to complain about the loud music.

From Danish news agency TV2:

Tivoli skruer op for lyden til ny sæson trods naboklager

Lydniveauet til udvalgte koncerter på Plænen i Tivoli hæves med syv decibel, når Tivoli lørdag åbner op for sin hidtil længste sommersæson.

Koncerterne i Tivoli kan fremover nydes syv decibel højere, når forlystelsesparken slår dørene op for sommersæsonen. Her ses Nile Rodgers på scenen i sommeren sidste år.

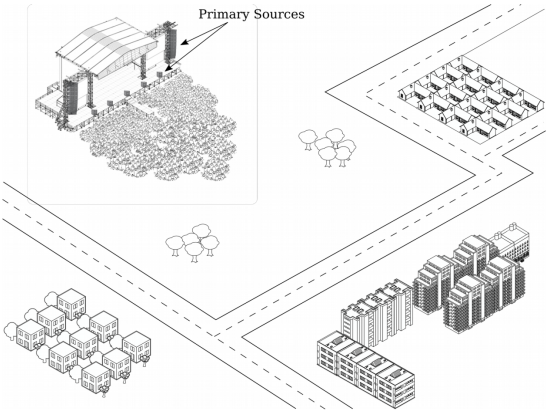
Foto: Torben Christensen - Ritzau Scanpix

21. mar 2018, kl. 13:33

https://www.tv2lorry.dk/artikel/tivoli-skruer-op-lyden-til-ny-saeson-trods-naboklager

A possible solution

Active sound cancellation from a secondary set of loudspeakers.



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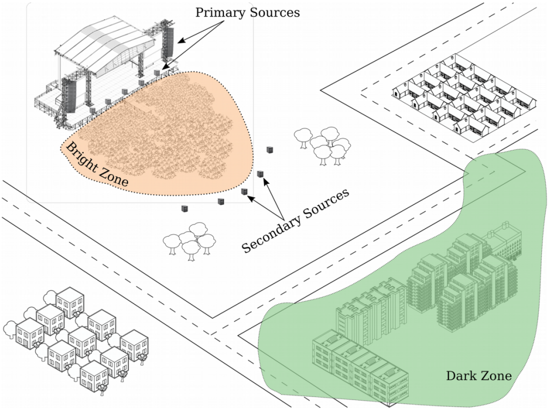

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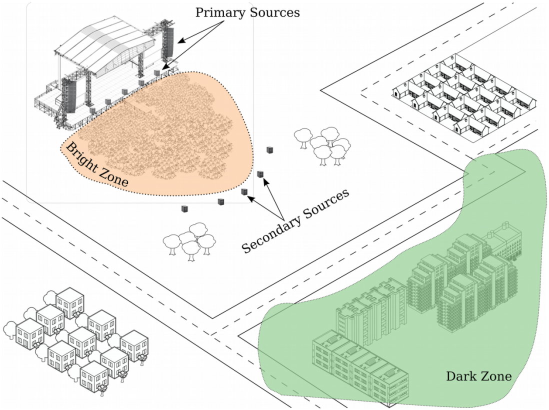
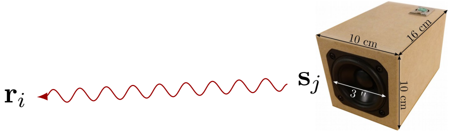


How do we model the sound waves from sources to the BZ and DZ?

A simple mathematical model

Assuming free-field conditions with monopole source.



Transfer function for each frequency f:

$$H_{ij} : \theta \mapsto (\theta_1 + \hat{\imath}\theta_2)\frac{\exp(\hat{\imath}kR_{ij})}{R_{ij}}$$

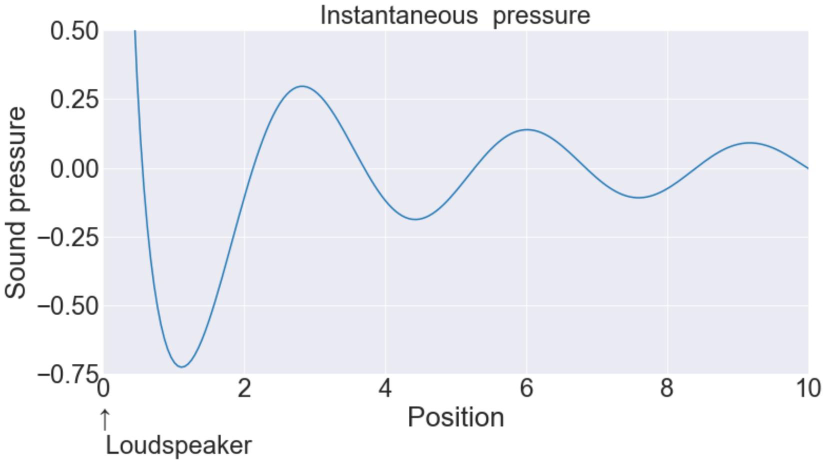
where $R_{ij} = \|\mathbf{r}_i - \mathbf{s}_j\|_2$, is the distance from source $\mathbf{s}_j$ to location $\mathbf{r}_i$ and $k = k(f)$ is the wave number.

A simple mathematical model: 1D Illustration

Transfer function for loudspeaker given $\theta = (0.65, 0.5)$ and $k = 2$.
We are plotting the instantaneous pressure:

$$\mathrm{Re}\left((\theta_1 + \hat{\imath}\theta_2)\frac{\exp(\hat{\imath}kR)}{R}\right)$$

.



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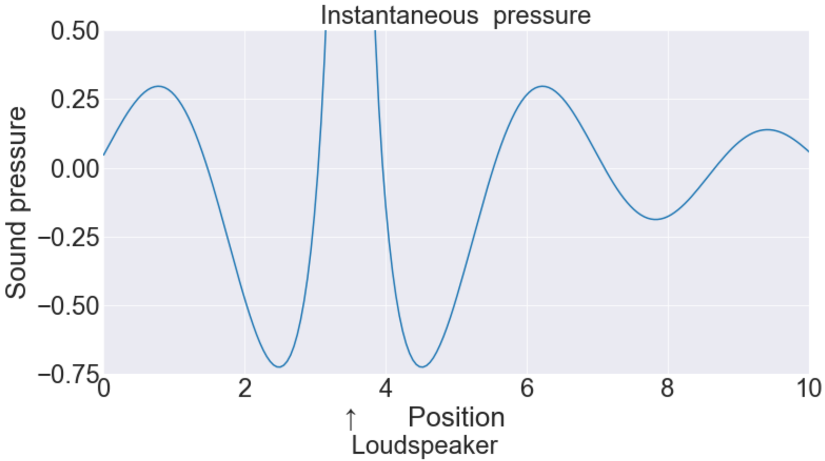
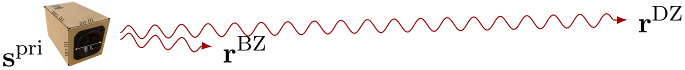


Sound field control illustrated



$$(\theta_1 + \hat{\imath}\theta_2)\frac{\exp(\hat{\imath}kR)}{R}$$

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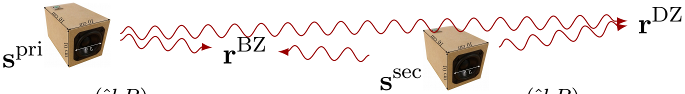
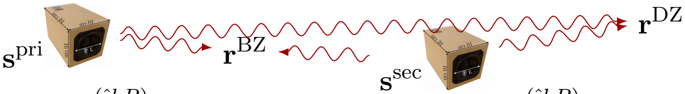


$$(\theta_1 + \hat{\imath}\theta_2)\frac{\exp(\hat{\imath}kR)}{R}$$

$$(w_1 + \hat{\imath}w_2)(\theta_1 + \hat{\imath}\theta_2)\frac{\exp(\hat{\imath}kR)}{R}$$

control filters

Sound field control illustrated



$(\theta_1 + \hat{\imath}\theta_2)\dfrac{\exp(\hat{\imath}kR)}{R}$ $\quad$ $(w_1 + \hat{\imath}w_2)(\theta_1 + \hat{\imath}\theta_2)\dfrac{\exp(\hat{\imath}kR)}{R}$

control filters

Define optimization problem to acquire control filters:

$$\min_{w} \|H_{\hat{\theta}}^{\mathrm{sec,BZ}} w\|_2^2 + \|H_{\hat{\theta}}^{sec,DZ} w + H_{\hat{\theta}}^{\mathrm{pri,DZ}} \mathbf{1}\|_2^2,$$

where $H_{\hat{\theta}}^{\mathbf{s},\mathbf{r}}$ of size $\#\mathrm{s} \times \#\mathbf{r}$ contain (estimated) the transfer functions for each combination of source s and location $\mathbf{r}$.

The notation pri and sec denotes all the primary and secondary sources and BZ and DZ are all points in the Bright and Dark Zone respectively.

Two problems

- Problem 1: Estimate model paramters $\hat{\theta}$ from measurements d

$$d_{ij} = (\theta_1 + \hat{\imath}\theta_2)\frac{\exp(\hat{\imath}kR_{ij})}{R_{ij}} + e_1 + \hat{\imath}e_2, \quad e_i \sim \mathcal{N}(0, \sigma^2 I), \tag{1}$$

  for all sources $\mathbf{s}_j$ and receivers $\mathbf{r}_i$.
  Here $i = 1, \ldots, n_{\mathrm{mic}}$ and $j = 1, \ldots, n_{\mathrm{LS}}$

- Problem 2: Estimate control filters w.

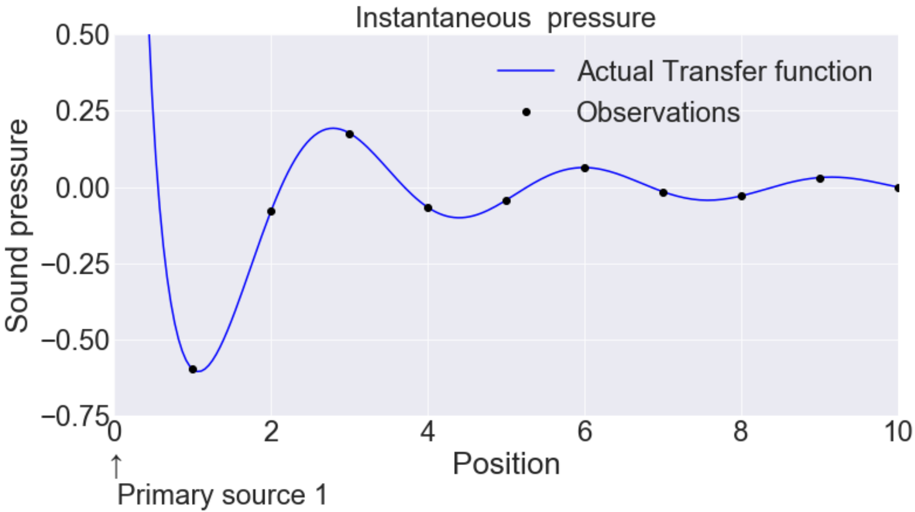
$$\min_w \|H_{\hat{\theta}}^{\mathrm{BZ}} w\|_2^2 + \|H_{\hat{\theta}}^{DZ} w + H_{\theta}^{\mathrm{DZ}}\mathbf{1}\|_2^2, \tag{2}$$

  where

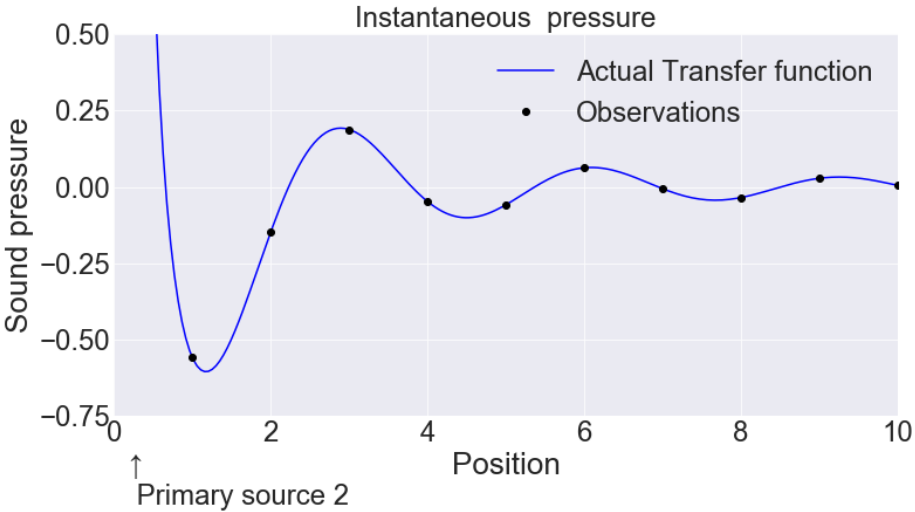
$$H_{kj} : (\theta_1 + \hat{\imath}\theta_2)\frac{\exp(\hat{\imath}kR_{kj}^*)}{R_{kj}^*}.$$

  Here $k = 1, \ldots, n_{\mathrm{cp}}$ and $j = 1, \ldots, n_{\mathrm{LS}}$

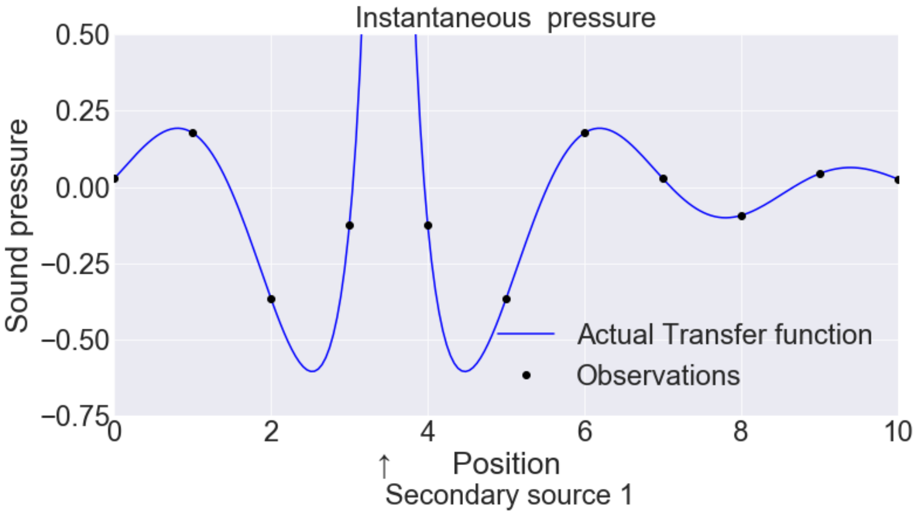
Example: Measured data



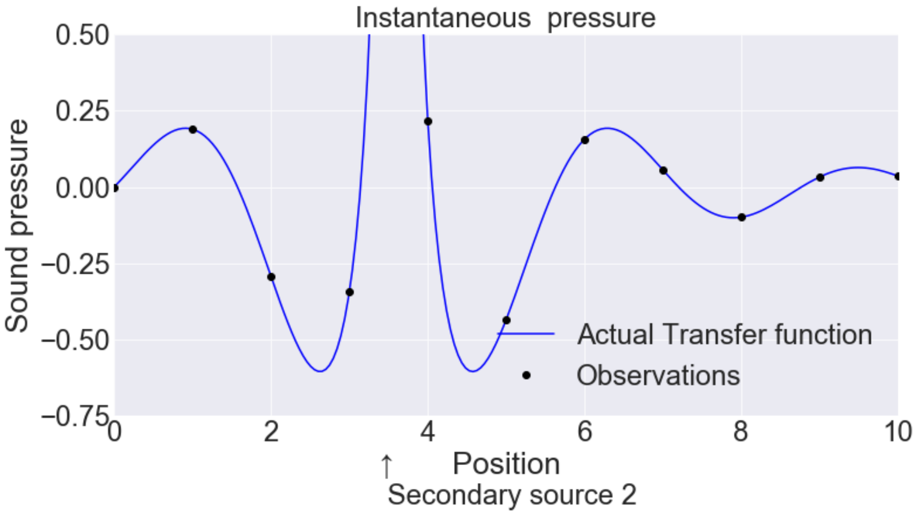
Example: Measured data



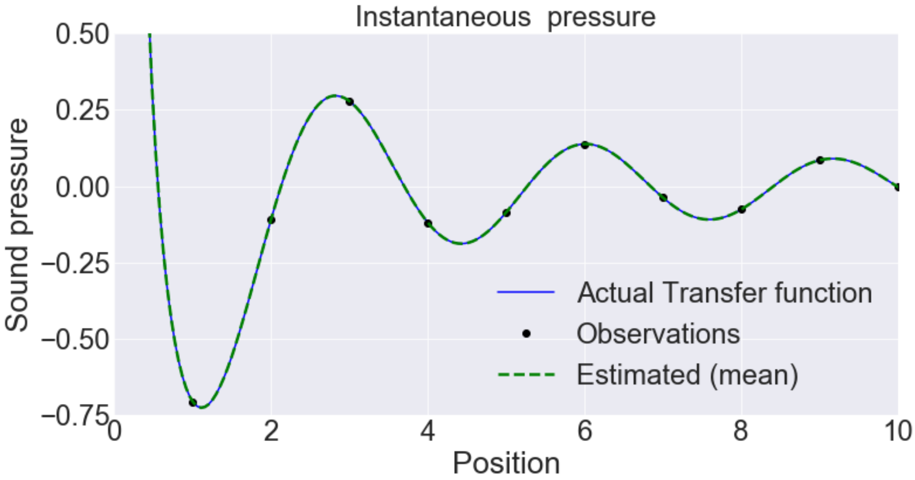
Example: Measured data



Example: Measured data



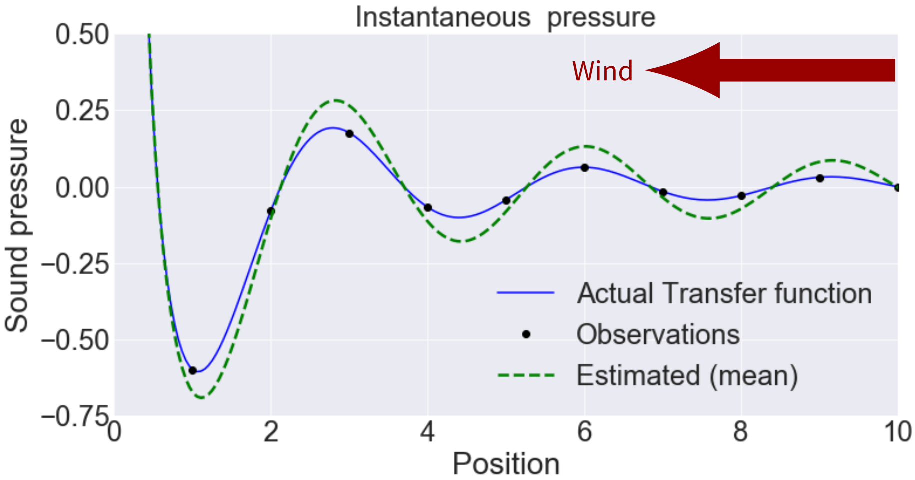
Example: Estimated transfer function



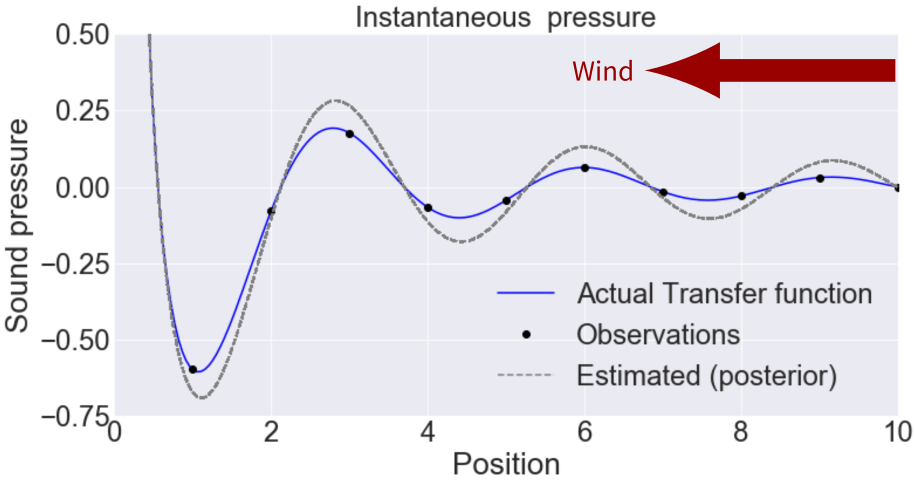
Example: Estimated transfer function

In outdoor concerts there may be many factors that influence the sound wave such as wind, temperature, reflections etc.

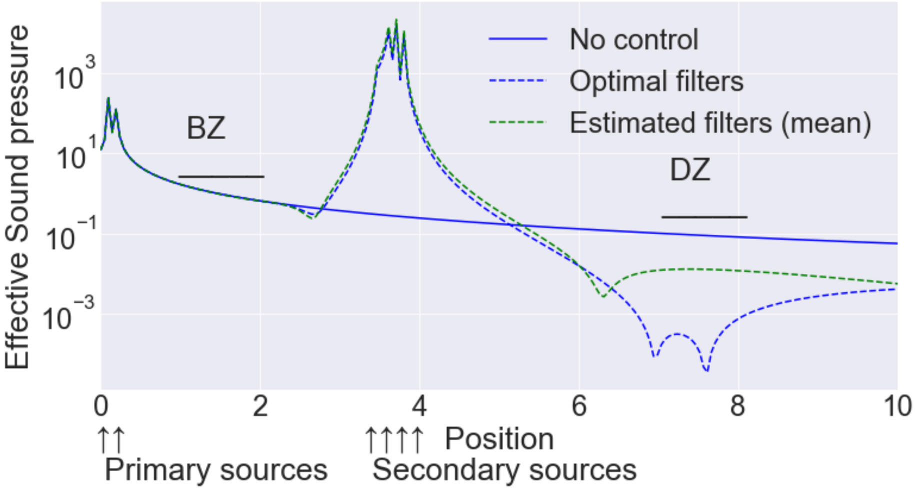
Example: Estimated transfer function



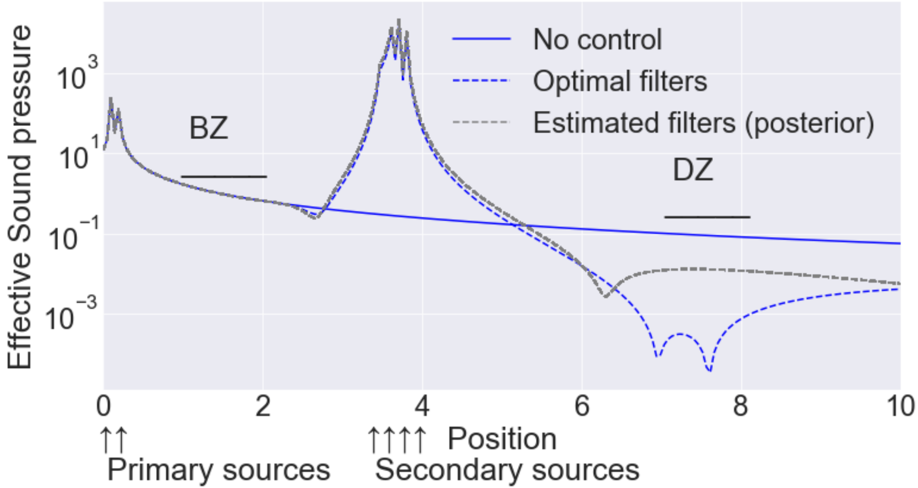
Example: Estimated transfer function



Example: Sound field control



Example: Sound field control



Including the model discrepancy using Gaussian Processes

- Problem 1: Estimate model parameters $\hat{\theta}, \delta$ from model

$$d_{ij} = (\theta_1 + \hat{\imath}\theta_2)\frac{\exp(\hat{\imath}kR_{ij})}{R_{ij}} + \delta^r_{R_{ij}} + \hat{\imath}\delta^{\hat{\imath}}_{R_{ij}} + e_1 + \hat{\imath}e_2, \quad e_i \sim \mathcal{CN}(0, \sigma^2 I), \tag{3}$$

for all sources $\mathbf{s}_j$ and receivers $\mathbf{r}_i$. Here $\delta_R \sim \mathcal{N}(0, K_R)$.
Here $i = 1, \ldots, n_{\mathrm{mic}}$ and $j = 1, \ldots, n_{\mathrm{LS}}$

- Problem 2: Estimate control filters w.

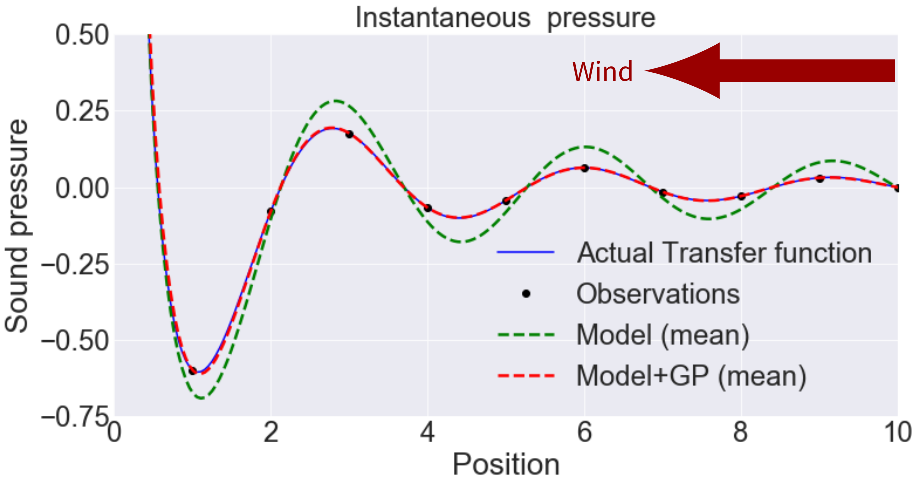
$$\min_w \|H^{\mathrm{BZ}}_{\hat{\theta}} w\|_2^2 + \|H^{DZ}_{\hat{\theta}} w + H^{\mathrm{DZ}}_{\theta}\mathbf{1}\|_2^2, \tag{4}$$

where

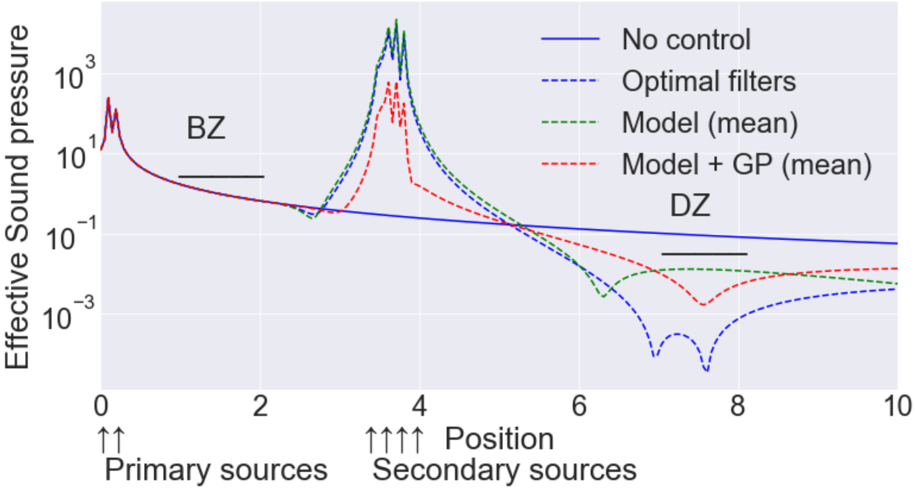
$$H_{kj} : (\theta_1 + \hat{\imath}\theta_2)\frac{\exp(\hat{\imath}kR^*_{kj})}{R^*_{kj}} + \delta^r_{R^*_{kj}} \mid R^*, R, \delta^r_R + \hat{\imath}\delta^{\hat{\imath}}_{R^*_{kj}} \mid R^*, R, \delta^{\hat{\imath}}_R$$

Here $k = 1, \ldots, n_{\mathrm{cp}}$ and $j = 1, \ldots, n_{\mathrm{LS}}$

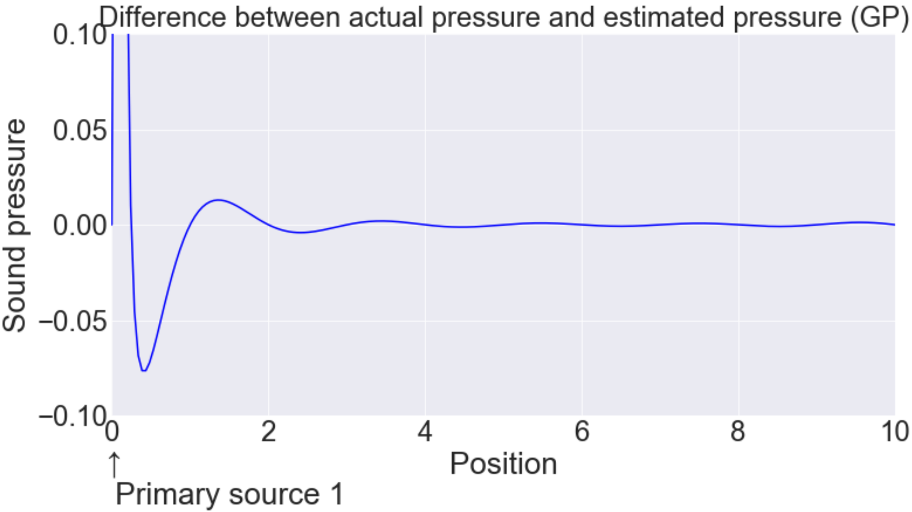
Example: Estimating model parameters (including GP)



Example: Sound field control (including GP)

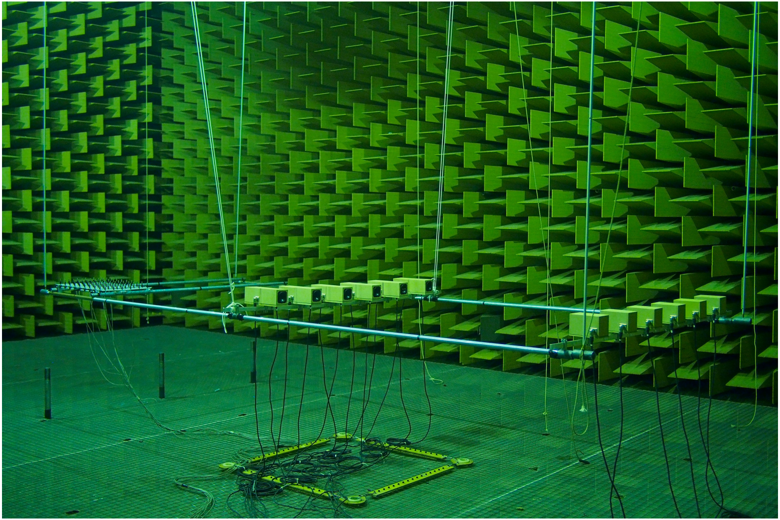


Why are the filters not optimal?

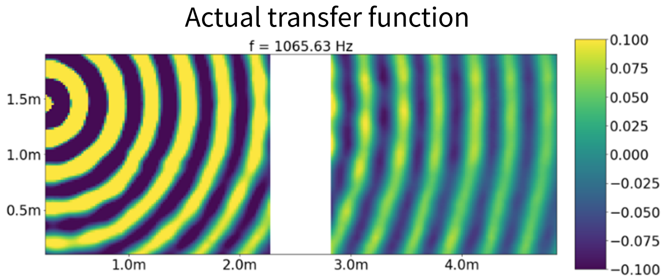


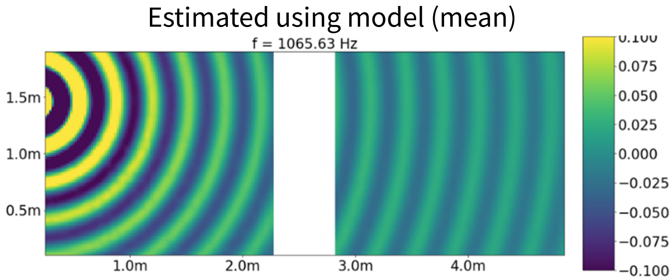
Results on real data

Sound field control in anechoic chamber



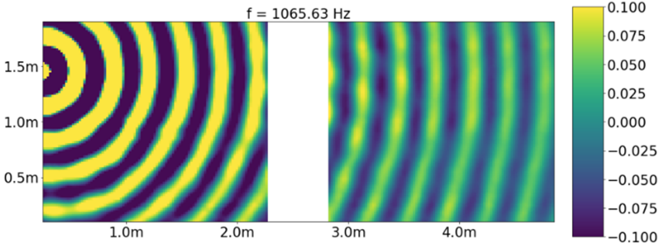
Results on real data



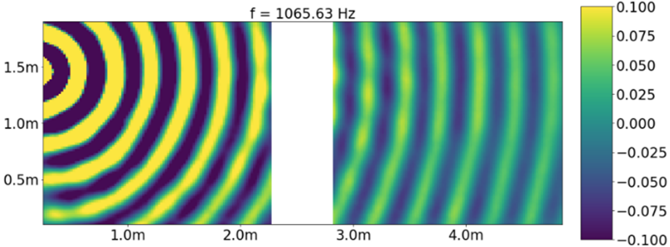


Results on real data

Actual transfer function



Estimated using model + GP (mean)



Sound field control: Conclusion and future work

- We are able to improve the model predictions and thus improve the sound field control by including a model discrepancy term described by a Gaussian Process
- Real world results show that the process works, but requires a lot of observations.

Future work:

- More accurate forward model so model discrepancy is less complex
  $\implies$ fewer observations needed.
- More specialized covariance functions to match the actual model discrepancy
  $\implies$ fewer observations needed.
- Non-Gaussian Processes?

References

[Bardsley 2018] J. Bardsley. Computational uncertainty quantification for inverse problems. SIAM, 2018.

[Brynjarsdóttir 2014] J. Brynjarsdóttir and A. O'Hagan. "Learning about Physical Parameters: the Importance of Model Discrepancy". Inverse Problems. 30.11 (2014): 114007.

[Kennedy 2001] M. C. Kennedy and A. O'Hagen. "Baysian calibration of computer models". J. R. Statist. Soc. B, 63.3 (2001): 425-464.

[Rasmussen 2006] C. E. Rasmussen and C. K. I. Williams. Gaussian Processes for Machine Learning. MIT Press, 2006.