Multi-resolution Multi-task Gaussian Processes

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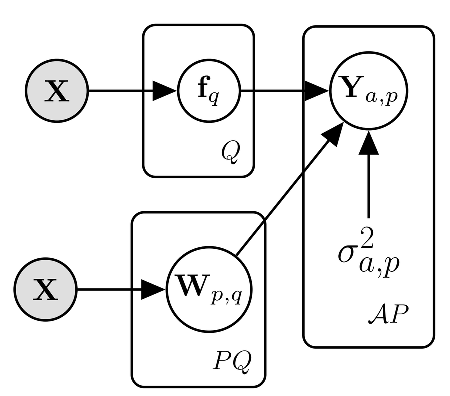
Introduction

- Consider integrating observations at varying spatio-temporal sampling resolutions (*multi-resolution*, MR), noise levels (*multi-fidelity*) and tasks
- Develop MR-GPRN that extends the Gaussian Process Regression Network (GPRN) of [4] to handle multi-resolution observations, additionally we utilise a composite likelihood to adjust posterior uncertainty under model misspecification
- Dervive MR-DGP that extends the Deep GP of [3] to handle multi-resolution data and any biases between the observation processes

Modelling Dependent Observations

- Construct $\mathcal{A}$ datasets $\{(\mathbf{X}_a, \mathbf{Y}_a)\}_{a=1}^{\mathcal{A}}$ where $\mathbf{Y}_a \in \mathbb{R}^{N_a \times P}$ for P tasks and N_a observations and $\mathbf{X}_a \in \mathbb{R}^{N_a \times |\mathcal{S}_a| \times D_a}$ over a (discretised) sampling area $\mathcal{S}_a$
- Introduce Q latent GPs $\mathbf{f}_q \sim \mathcal{GP}(0, \mathbf{K}_q)$ and PQ task-specific GPs $\mathbf{W}_{p,q} \sim \mathcal{GP}(0, \mathbf{K}_{p,q})$. Link these to the different resolutions through the likelihood:

$$p(\mathbf{Y}|\mathbf{W}, \mathbf{f}) = \prod_{a=1}^{\mathcal{A}} \prod_{p=1}^{P} \prod_{n=1}^{N_a} \mathcal{N}(\mathbf{Y}_{a,p,n} | \frac{1}{|\mathcal{S}_a|} \int_{\mathcal{S}_{a,n}} \sum_{q=1}^{Q} \mathbf{W}_{p,q}(\mathbf{x}) \odot \mathbf{f}_q(\mathbf{x})\, d\mathbf{x}, \sigma^2_{a,p}\mathbf{I})^{\phi}$$



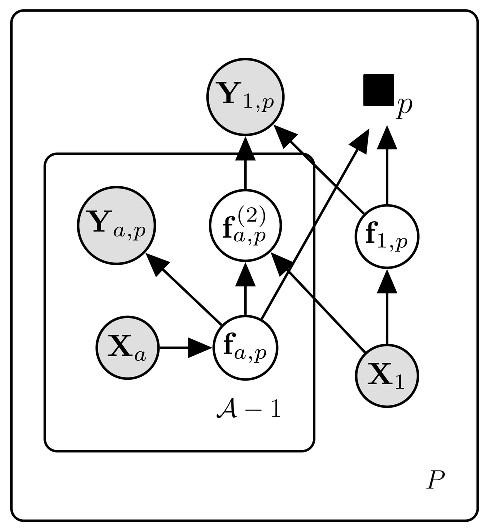
Algorithm 1: Inference of MR-GPRN

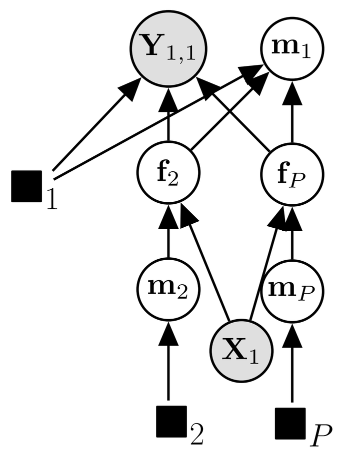
Input: $\{(\mathbf{X}_a, \mathbf{Y}_a)\}_{a=1}^{\mathcal{A}}$, initial θ,
$\hat{\theta} \leftarrow \arg\max_{\theta} \sum_{a=1}^{\mathcal{A}} \ell(\mathbf{Y}_a|\theta)$
$\mathbf{H} \leftarrow \sum_{a=1}^{\mathcal{A}} (\nabla \ell(\mathbf{Y}_a|\hat{\theta})(\nabla \ell(\mathbf{Y}_a|\hat{\theta}))^T$
$\mathbf{J} \leftarrow \nabla^2 \ell(\mathbf{Y}|\hat{\theta})$
$\phi \leftarrow \begin{cases} \frac{|\hat{\theta}|}{\mathrm{Tr}[\mathbf{H}(\hat{\theta})^{-1}\mathbf{J}(\hat{\theta})]} \\ \frac{\mathrm{Tr}[\mathbf{H}(\hat{\theta})\mathbf{J}(\hat{\theta})^{-1}\mathbf{H}(\hat{\theta})]}{\mathrm{Tr}[\mathbf{H}(\hat{\theta})]} \end{cases}$
$\theta_1 \leftarrow \arg\min_{\theta} \left(\sum_{a=1}^{\mathcal{A}} \phi \mathbb{E}_q \left[\ell(\mathbf{Y}_a|\theta)\right] + \mathcal{KL}\right)$

Modelling Biased Observations

- We assume that the highest resolution is the observation of interest and learn the mapping and calibration from the lower resolution observations
- A mixture of DGP experts allows for non-overlapping datasets

- Each $\mathbf{f}^{(\cdot)}{}_{a,p} \sim \mathcal{GP}(0, \mathbf{K}^{(\cdot)}{}_{a,p})$
- $\mathbf{m}_p = \sum_{a=1}^{\mathcal{A}} \beta_a \odot \mathbf{f}^{(\cdot)}_{a,p}$
- $\beta_a = (1 - \mathbf{V}_a) \sum_i^a \mathbf{V}_i$

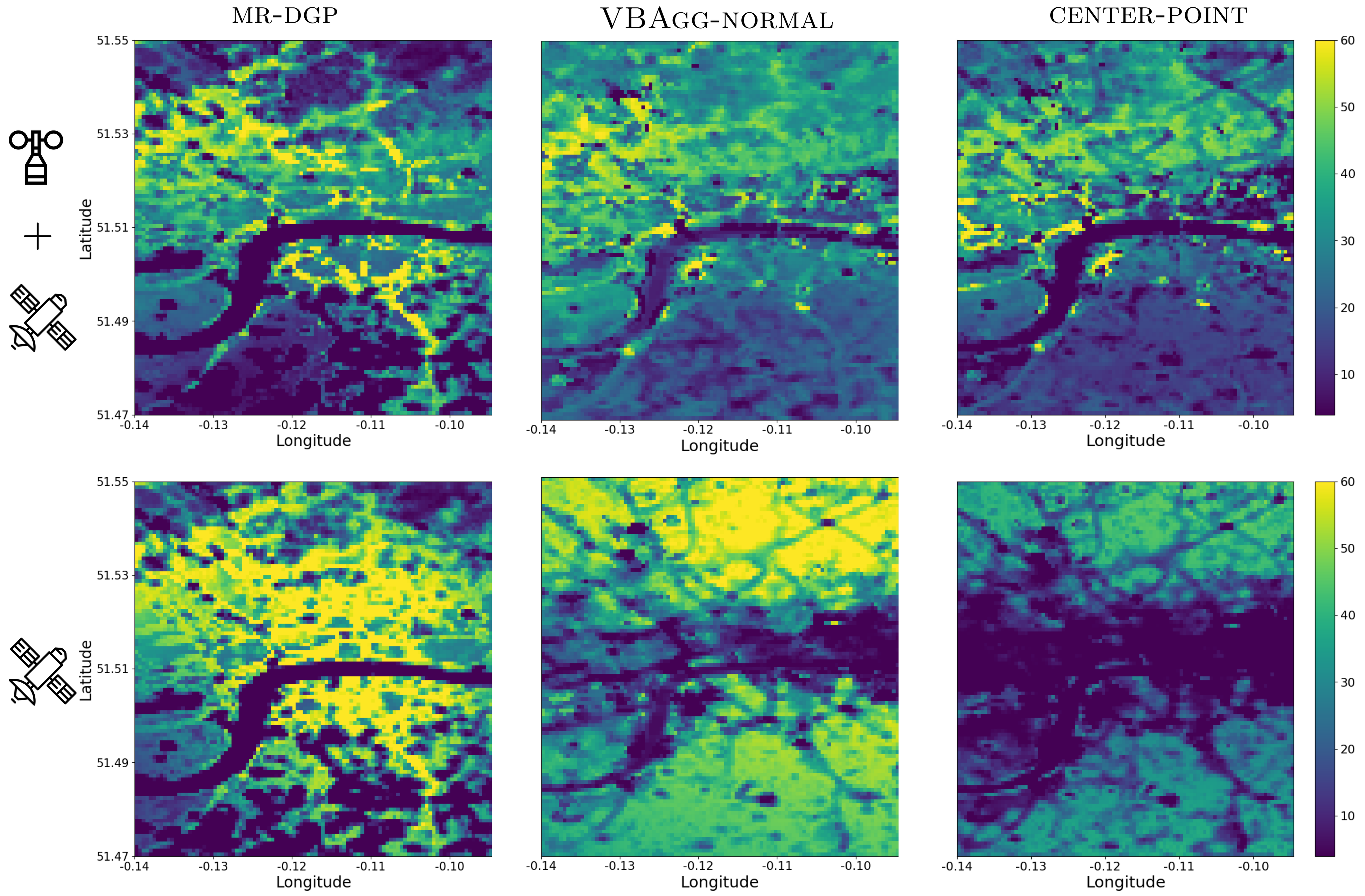




- Each likelihood has its own noise term allowing for multi-fidelity learning
- Propagating samples allows predictions at all resolutions and tasks

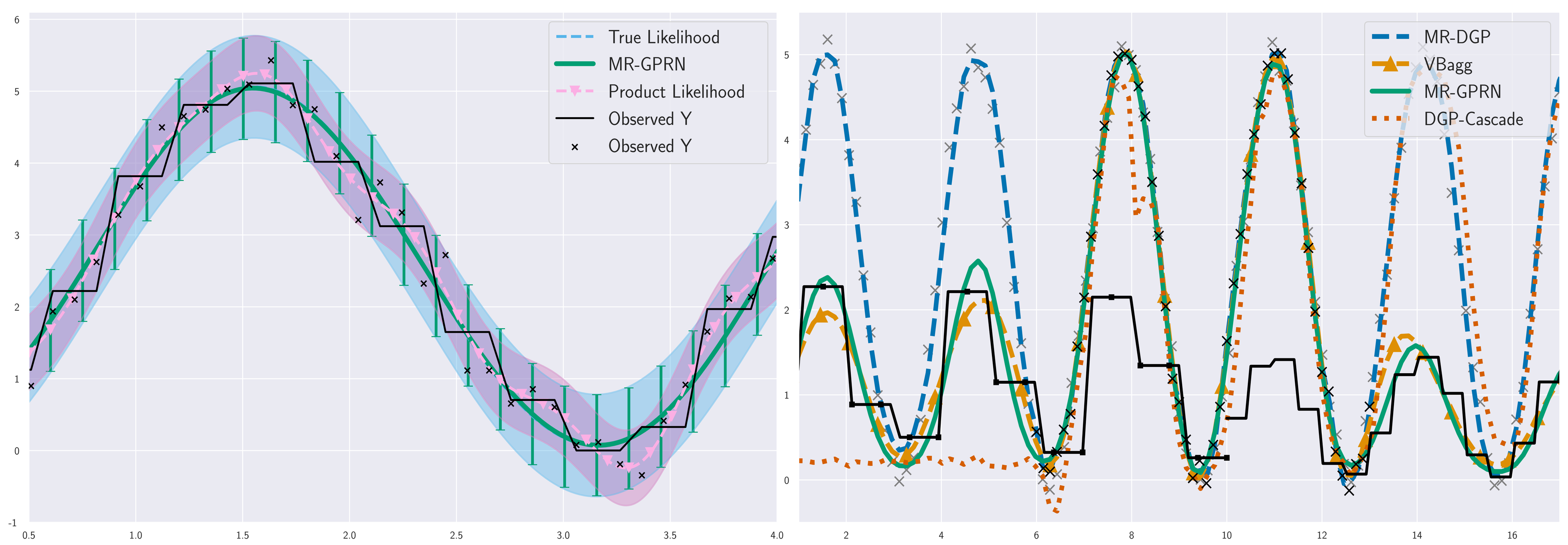
Forecasting NO_2 Across London

- Spatio-temporal estimation and forecasting of NO_2 levels in London



- **Top row**: Spatial slices with observations from both LAQN and the satellite model (low spatial resolution) are present. All models are able to capture the high resolution structure
- **Bottom row**: Spatial slices from the same models where *only* observations from the satellite model are present. Only MR-DGP retains the high resolution structure

Biased and Dependent Observations



- **Left**: MR-GPRN corrects for model misspecification from a product likelihood through the use of a composite likelihood
- **Right**: MR-DGP learns a scaling bias between multi-resolution datasets allowing the true predictive mean to be recovered instead of resorting to the uncalibrated observations. Whereas DGP-Cascade is unable to handle the non-overlapping multi-resolution datasets

Variational Lower Bounds

- For MR-GPRN we derive efficient closed form variational lower bounds. We augment all latent GPs with inducing points and derive the ELL:

$$\mathrm{ELL}_{a,p,n,k} = \pi_k \log \mathcal{N}\left(Y_{a,p,n} \mid \frac{1}{|\mathcal{S}_{a,n}|} \sum_{\mathbf{x} \in \mathcal{S}_{a,n}} \sum_{q=1}^{Q} \boldsymbol{\mu}^{(w)}_{k,p,q}(\mathbf{x}) \boldsymbol{\mu}^{(f)}_{k,q}(\mathbf{x}), \sigma^2_{a,p}\right)$$
$$- \frac{\pi_k}{2\sigma^2_{a,p}} \frac{1}{|S_{a,n}|^2} \sum_{q=1}^{Q} \sum_{\mathbf{x}_1,\mathbf{x}_2} \boldsymbol{\Sigma}^{(w)}_{k,p,q} \boldsymbol{\Sigma}^{(f)}_{k,q} + \boldsymbol{\mu}^{(f)}_{k,q}(\mathbf{x}_1) \boldsymbol{\Sigma}^{(w)}_{k,p,q} \boldsymbol{\mu}^{(f)}_{k,q}(\mathbf{x}_2) \boldsymbol{\mu}^{(w)}_{k,p,q}(\mathbf{x}_1) \boldsymbol{\Sigma}^{(f)}_{k,q} \boldsymbol{\mu}^{(w)}_{k,p,q}(\mathbf{x}_2)$$

- For MR-DGP we sample from the base GPs and propagate the samples up:

$$q(\mathbf{m}^*_1) = \int q(\mathbf{m}^*_1 | \mathrm{Pa}(\mathbf{m}^*_1)) \prod_{\mathbf{f} \in \mathrm{Pa}(\mathbf{m}^*_1)} q(\mathbf{f})\, d\mathrm{Pa}(\mathbf{m}^*_1) \approx \frac{1}{S} \sum_{s=1}^{S} q(\mathbf{m}^*_1 | \{\mathbf{f}^{(s)}\}_{\mathbf{f} \in \mathrm{Pa}(\mathbf{m}^*_1)})$$

Results

Biased Mean

Model	RMSE	MAPE
MR-CASCADE	2.12	0.16
VBAgg-normal	1.68	0.14
MR-GPRN	1.6	0.14
MR-DGP	**0.19**	**0.02**

NO2 Across London

Model	RMSE	MAPE
Single GP	20.55 ± 9.44	0.8 ± 0.16
center-point	18.74 ± 12.65	0.65 ± 0.21
VBAgg-normal	16.16 ± 9.44	0.69 ± 0.37
MR-GPRN w/o CL	12.97 ± 9.22	0.56 ± 0.32
MR-GPRN w CL	11.92 ± 6.8	0.45 ± 0.17
MR-DGP	$\mathbf{6.27 \pm 2.77}$	$\mathbf{0.38 \pm 0.32}$

- MR-DGP is able to substantially outperform both VBAgg-normal, MR-GPRN
- MR-DGP can handle biases between observation processes

Future Work

- Incorporate physical constraints in latent space through physics-informed machine learning
- Reduce computational complexity through state-space GP formulations
- Explore further model robustness through recent advances in Generalised Variance Inference [5]
- Explore further MR constructions e.g. the concurrent submissions [6, 7]

Key References

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CODE

PAPER

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