# Learning on Aggregate Outputs with Kernels

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# Gaussian Processes

Consider function values $\mathbf{f} = (f(x_1), \ldots, f(x_n))^\top$ at a set of inputs, and observations $\mathbf{y} = (y_1, \ldots, y_n)$. GP regression model is given by

$$\mathbf{f} \sim \mathcal{N}(0, \mathbf{K})$$
$$\mathbf{y}|\mathbf{f} \sim \mathcal{N}(\mathbf{f}, \sigma^2 I)$$

where $\mathbf{K}$ is the (covariance) kernel matrix on inputs.

- Posterior distribution:

$$\mathbf{f}|\mathbf{y} \sim \mathcal{N}(\mathbf{K}(\mathbf{K} + \sigma^2 I)^{-1}\mathbf{y}, \mathbf{K} - \mathbf{K}(\mathbf{K} + \sigma^2 I)^{-1}\mathbf{K})$$

- **Posterior predictive distribution**: Suppose $\mathbf{x}'$ is an unseen test set. We can extend our model to include the function values $\mathbf{f}'$ at the test set:

$$\begin{pmatrix} \mathbf{y} \\ \mathbf{f}' \end{pmatrix} \sim \mathcal{N}\left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \mathbf{K_{xx}} + \sigma^2 I & \mathbf{K_{xx'}} \\ \mathbf{K_{x'x}} & \mathbf{K_{x'x'}} \end{pmatrix} \right)$$

  where $\mathbf{K_{xx'}}$ is matrix with $(i, j)$-th entry $k(x_i, x'_j)$.
- Basic Gaussian conditioning gives:

$$\mathbf{f}'|\mathbf{y} \sim \mathcal{N}\left(\mathbf{K_{x'x}}(\mathbf{K_{xx}} + \sigma^2 I)^{-1}\mathbf{y}, \mathbf{K_{x'x'}} - \mathbf{K_{x'x}}(\mathbf{K_{xx}} + \sigma^2 I)^{-1}\mathbf{K_{xx'}}\right).$$

# Non-Gaussian observation models

Consider function values $\mathbf{f} = (f(x_1), \ldots, f(x_n))^\top$ at a set of inputs, and observations $\mathbf{y} = (y_1, \ldots, y_n)$, with a general observation model

$$\mathbf{f} \sim \mathcal{N}(0, \mathbf{K})$$

$$\mathbf{y}|\mathbf{f} \sim p(\mathbf{y}|\mathbf{f}) = \prod_{i=1}^{n} p\left(y_i|f(x_i)\right).$$

- Posterior distribution $p(\mathbf{f}|\mathbf{y})$ is no longer tractable.
- **Variational approximation**: write $q(\mathbf{f}) = \mathcal{N}(\mathbf{f}|\mu, \Sigma)$ and learn $\mu$, $\Sigma$ by optimizing the evidence lower bound (ELBO):

$$\mathcal{L}(\mu, \Sigma) = \mathbb{E}_q \log p(\mathbf{y}|\mathbf{f}) - \underbrace{KL\left(q(\mathbf{f})||p(\mathbf{f})\right)}_{\text{tractable}}$$

- **Inducing points / landmarks**: often coupled with a scalable GP approximation, taking $m \ll n$ inducing inputs $z_1, \ldots, z_m$ and respective values $\mathbf{u} = (f(z_1), \ldots, f(z_m))$, with a joint variational posterior $q(\mathbf{f}, \mathbf{u}) = p(\mathbf{f}|\mathbf{u})q(\mathbf{u})$, so that only variational parameters of $q(\mathbf{u})$ need to be inferred.

# GP regression and Kernel Ridge Regression

If KRR and GPR use the same kernel and if the regularization parameter $\lambda$ equals the noise variance $\sigma^2$, KRR estimate of the function coincides with the GPR posterior mean/mode. Indeed, recall that in KRR we are solving empirical risk minimisation

$$\min_{f \in \mathcal{H}_k} \sum_{i=1}^{n} \left(y_i - f(x_i)\right)^2 + \sigma^2 \left\|f\right\|_{\mathcal{H}_k}^2 ,$$

and are fitting a function of the form $f(x) = \sum_{i=1}^{n} \alpha_i k\left(\cdot, x_i\right)$. Closed form solution is given by $\alpha = \left(\mathbf{K_{xx}} + \sigma^2 I\right)^{-1} \mathbf{y}$. But then if we wish to predict function values at a new set $\mathbf{x}' = \{x'_j\}_{j=1}^{m}$ of input vectors, we have

$$f(x'_j) = \sum_{i=1}^{n} \alpha_i k\left(x'_j, x_i\right) = \left[k(x'_j, x_1), \ldots, k(x'_j, x_n)\right] \left(\mathbf{K_{xx}} + \sigma^2 I\right)^{-1} \mathbf{y},$$

and $\left[k(x'_j, x_1), \ldots, k(x'_j, x_n)\right]$ is the $j$-th row of $\mathbf{K_{x'x}}$.
More generally, GP posterior mode for any likelihood model lies in the RKHS (essentially the same proof as the representer theorem).

# GPs and RKHSs: shared mathematical foundations

- The same notion of a (positive definite) kernel, but conceptual gaps between communities.
- Orthogonal projection in RKHS $\Leftrightarrow$ Conditioning in GPs.
- Beware! 0/1 laws: GP sample paths with (infinite-dimensional) covariance kernel $k$ almost surely fall outside of $\mathcal{H}_k$.
  - But the space of sample paths is only slightly larger than $\mathcal{H}_k$ (outer shell).
  - It is typically also an RKHS (with another kernel).
- Worst-case in RKHS $\Leftrightarrow$ Average-case in GPs.

$$\mathrm{MMD}^2(P, Q; \mathcal{H}_k) = \left( \sup_{\|f\|_{\mathcal{H}_k} \leq 1} (Pf - Qf) \right)^2 = \mathbb{E}_{\mathrm{f} \sim \mathcal{GP}(0,k)} \left[ (P\mathrm{f} - Q\mathrm{f})^2 \right].$$

Radford Neal, 1998: "*prior beliefs regarding the true function being modeled and expectations regarding the properties of the best predictor for this function [...] need not be at all similar.*"

Gaussian Processes and Kernel Methods: A Review on Connections and Equivalences
M. Kanagawa, P. Hennig, DS, and B. K. Sriperumbudur
**ArXiv e-prints:1807.02582**
https://arxiv.org/abs/1807.02582

# Learning on Aggregate Outputs

# Motivation- Disease modelling

Suppose you have a country with $n$ regions and data on:

- number of malaria incidences per region (low resolution)
- many covariates per region (high resolution)

**Goal:** Predict malaria incidences at a higher resolution, given low resolution label data and high definition covariate data.

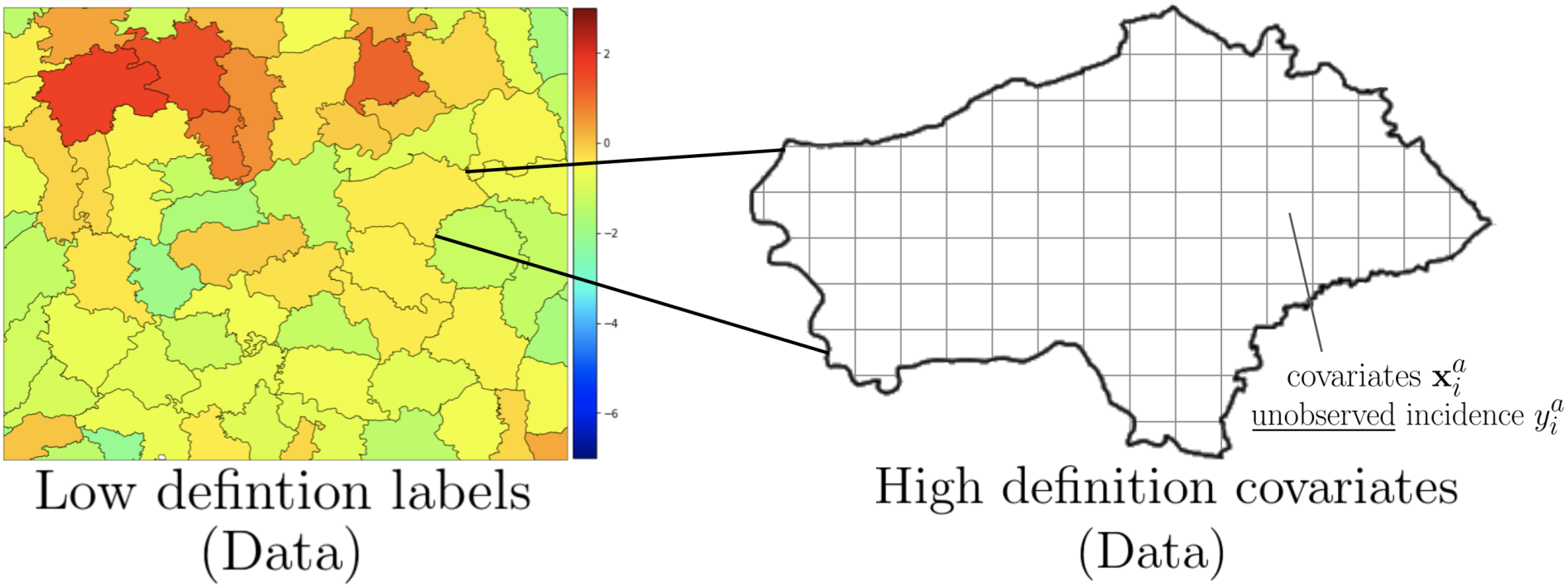


Figure: Log incidence rate of malaria

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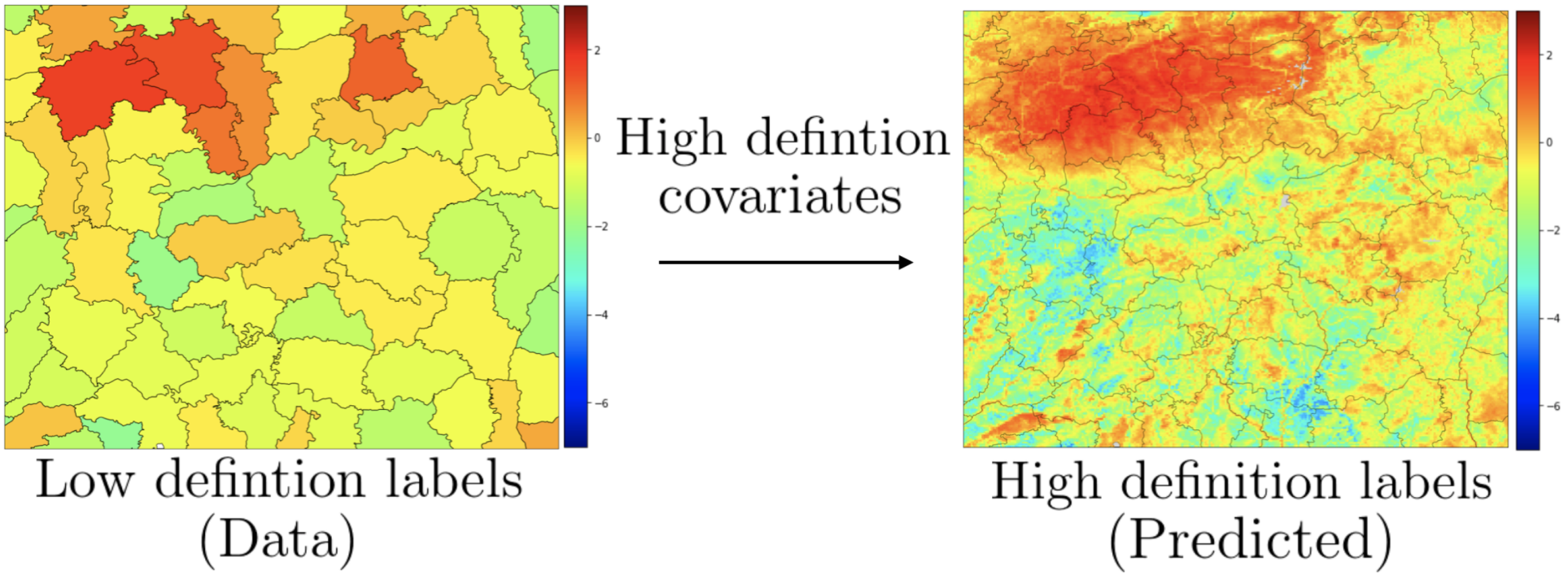



Figure: Log incidence rate of malaria

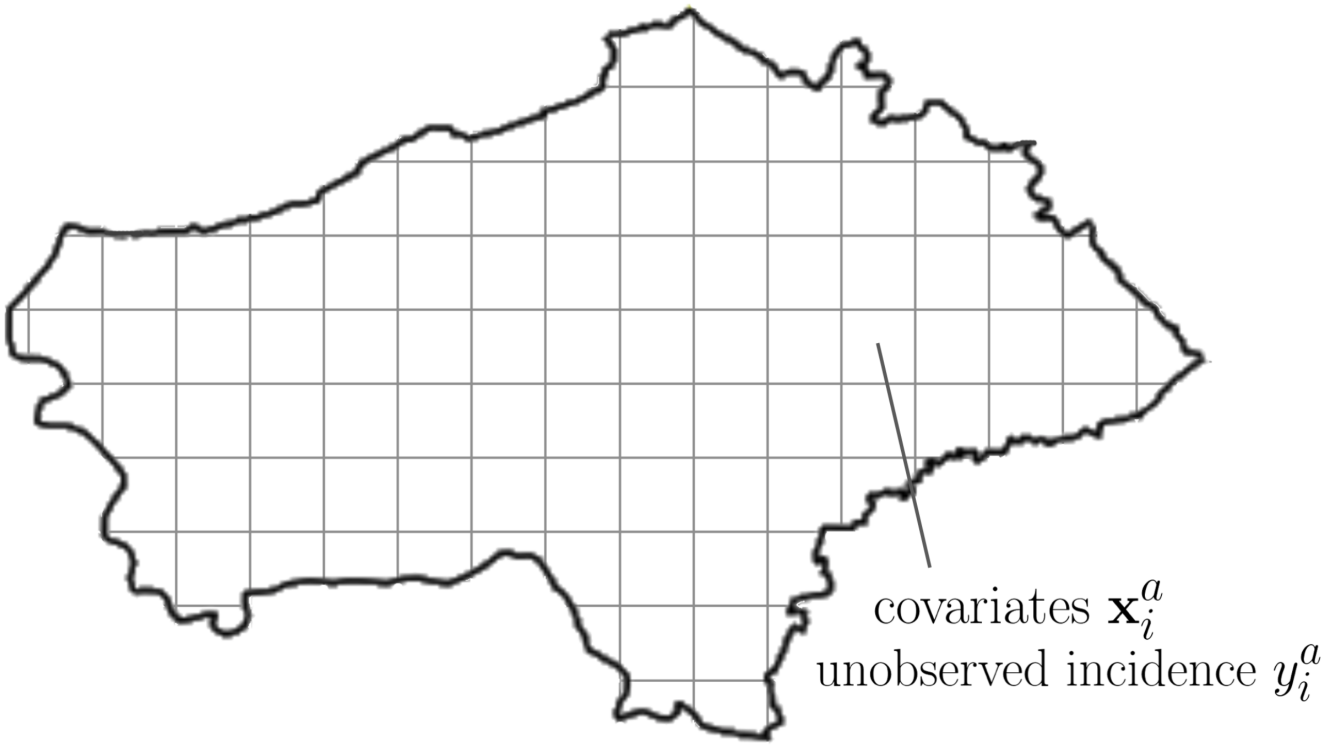
# Setup

Formally, we have $n$ regions, and for each region $a$, we have $N_a$ pixels (1km by 1km regions):

$$\text{Data: } (\{\mathbf{x}_i^1\}_{i=1}^{N_1}, y^1), \ldots, (\{\mathbf{x}_i^n\}_{i=1}^{N_n}, y^n)$$

- $\mathbf{x}_i^a$ is the covariates for the $i^{th}$ pixel of region $a$
- $y^a$ is the total observed incidence for region $a$

**Goal:** Predict $y_i^a$, the unknown incidence for pixel $i$ in region $a$.



# Learning on Aggregates

- *Supervised learning*: obtaining inputs has a lower cost than obtaining outputs/labels, hence we build a (predictive) functional relationship or a conditional probabilistic model of outputs given inputs.
- *Semisupervised learning*: because of the lower cost, there is much more unlabelled than labelled inputs.
- *Weakly supervised learning on aggregates*: because of the lower cost, inputs are at a much higher resolution than outputs.

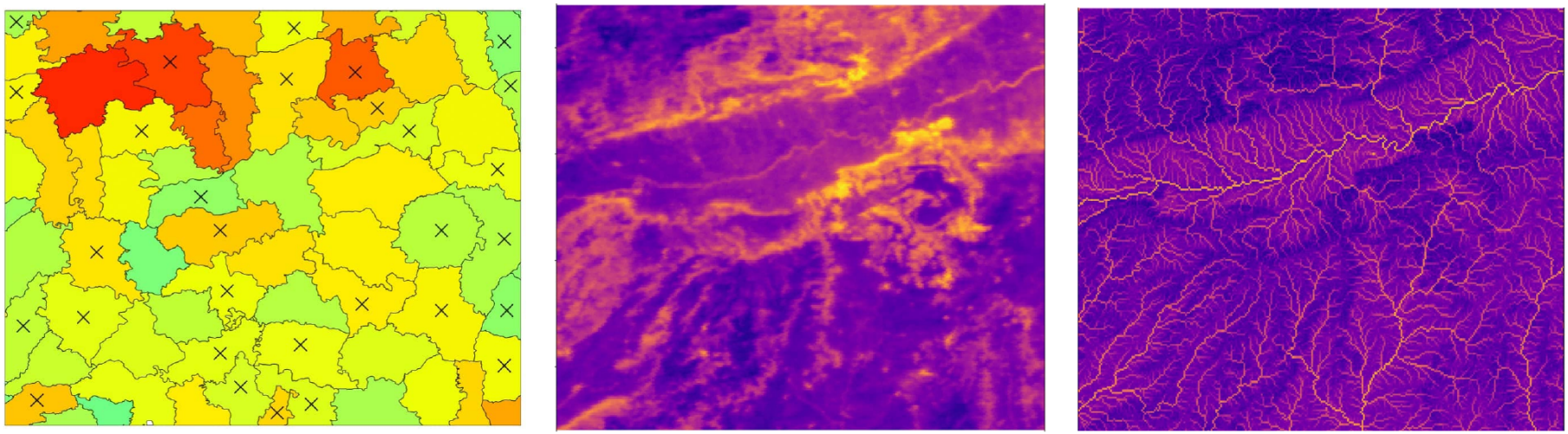
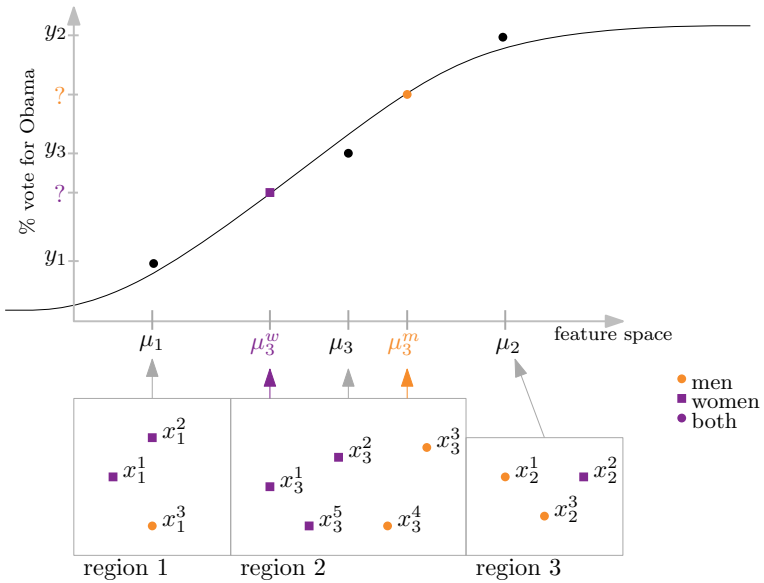
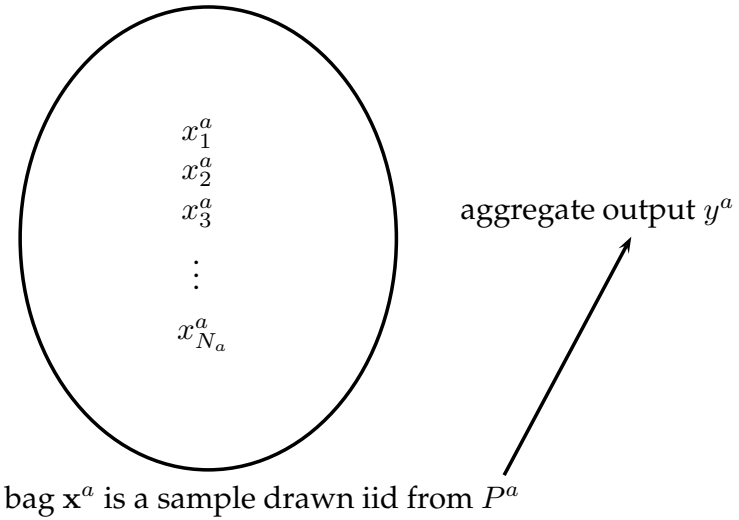


Figure: **left**: Malaria incidences reported per administrative unit; **centre**: land surface temperature at night; **centre**: topographic wetness index

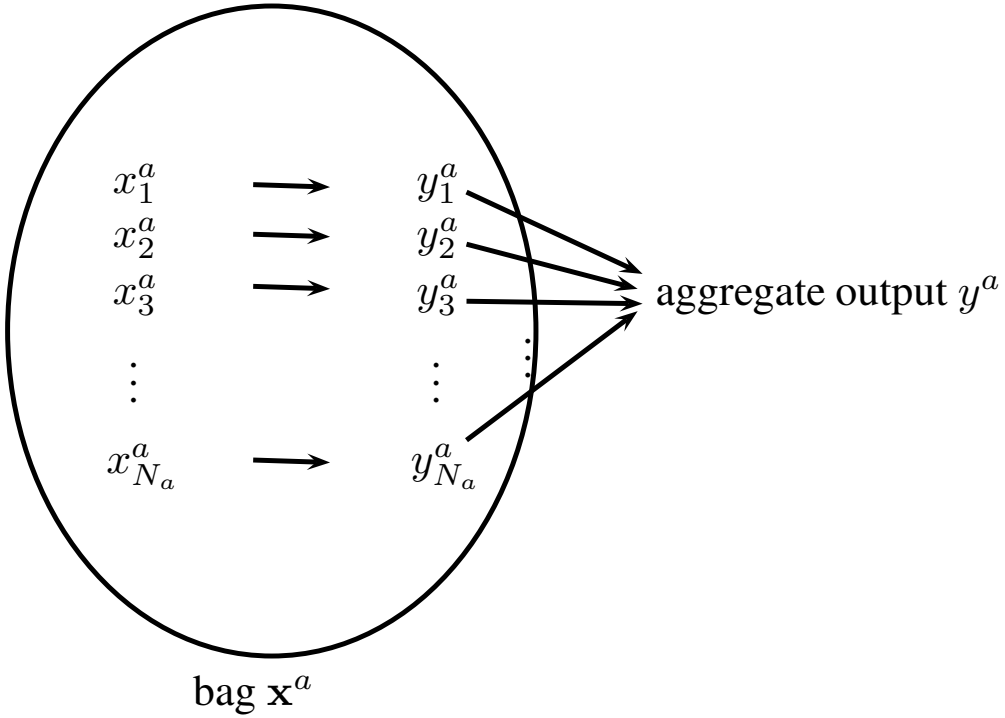
# Distribution regression: train on bags, predict on bags




- Distribution regression [Szabo et al 2015, Flaxman et al 2015, Law et al 2018]. An RKHS-based framework for learning on *bag inputs*: ecological inference, semi-automatic ABC,...
- Represents input bags using the (empirical) kernel mean embeddings $\hat{\mu}_a = \sum_{i=1}^{N_a} k(\cdot, \mathbf{x}_i^a)$.
- Individual labels need not exist - the label is a function of the whole population, e.g. a function of the parameters of the $a$-th sampling distribution.
- Individual predictions using RKHS-valued features of individual inputs? Covariate shift.

# Output disaggregation: train on bags, predict on individuals




- *Weakly supervised* ML problem. Classification instance widely studied in ML (*learning with label proportions*) [Quadrianto et al, 2009; Yu et al, 2013], but little work on regression / other observation likelihoods.
- Spatial statistics: 'down-scaling', 'fine-scale modelling' or 'spatial disaggregation' in the analysis of disease mapping, agricultural data, and species distribution modelling, but mostly simple linear models.
- This work: scalable variational GP machinery + general aggregation model.

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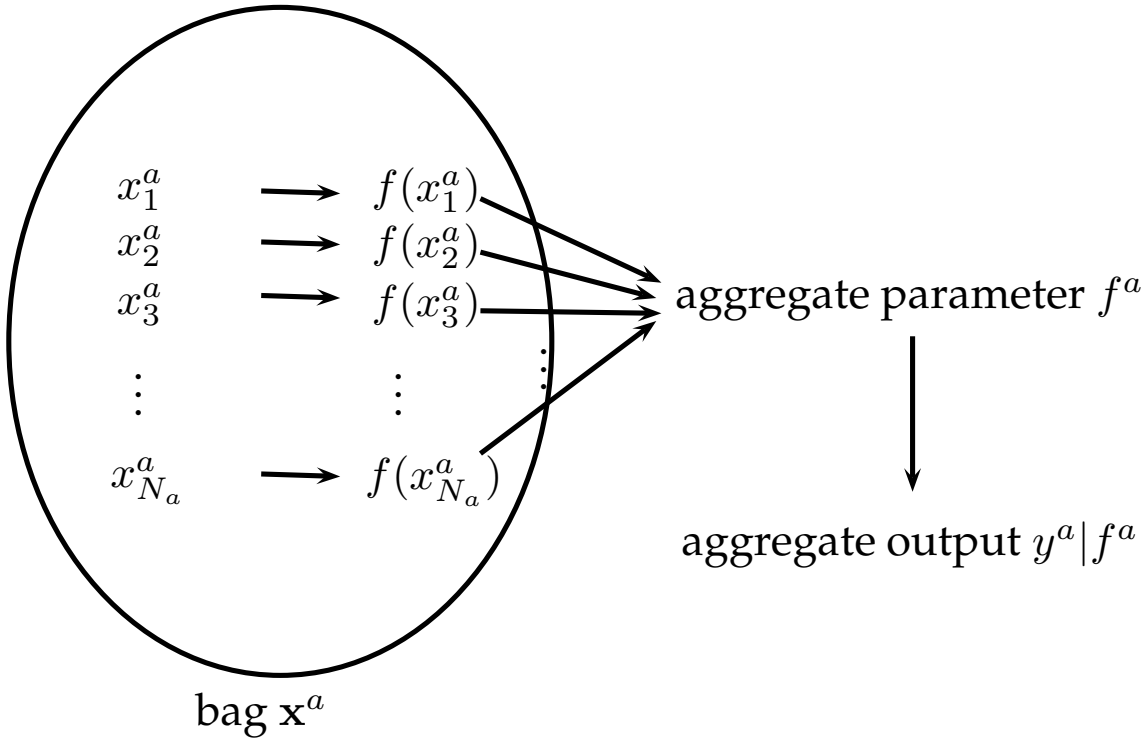


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# Bag Observation Model: Aggregation in Mean Parameters

- An exponential family model $p(y|\eta)$ for output $y \in \mathcal{Y}$, with mean parameter $\eta = \eta(x)$ depending on the individual input $x \in \mathcal{X}$.
- Given a fixed set of points $x_i^a \in \mathcal{X}$ such that $\mathbf{x}^a = \{x_1^a, \ldots, x_{N_a}^a\}$, i.e. a *bag* of points with $N_a$ *individuals*
- Observe the *aggregate outputs* for each of the bags: training data $(\{x_i^1\}_{i=1}^{N_1}, y^1), \ldots (\{x_i^n\}_{i=1}^{N_n}, y^n)$.
- However, we wish to estimate the regression value $\eta(x_i^a)$ for each individual (in-sample or out-of-sample), not for new bags.
- No restrictions on the collection of the individuals, with the bagging process possibly dependent on covariates $x_i^a$.

To relate the aggregate $y^a$ and the bag $\mathbf{x}^a = (x_i^a)_{i=1}^{N_a}$, we use the following *bag observation model*:

$$y^a|\mathbf{x}^a \sim p(y|\eta^a), \qquad \eta^a = \sum_{i=1}^{N_a} p_i^a \eta(x_i^a), \tag{1}$$

where $p_i^a$ is an optional fixed non-negative weight used to adjust the scales. .

# Poisson bag model: Modelling aggregate counts

The total observed incidence (of region $a$) $y^a$ is assumed to follow

$$y^a|\mathbf{x}^a \sim \text{Poisson}(p^a\lambda^a), \quad \lambda^a := \sum_{i=1}^{N_a} \frac{p_i^a}{p^a}\lambda(\mathbf{x}_i^a).$$

where $p_i^a$ is the population for pixel $i$ for region $a$ and $\lambda(\mathbf{x}_i^a)$ is a model on covariates and is the intended goal.

This model also implies that the unobserved pixel incidences follows:

$$y_i^a \sim \text{Poisson}(y_i^a|p_i^a\lambda(x_i^a))$$

Potential model formulation for $\lambda(\cdot)$:

- Neural network
- **Gaussian process**

# Gaussian process

For $\lambda(\cdot)$, we use a Gaussian Process (GP):

$$\lambda(\mathbf{x}_i^a) = \Psi(f(\mathbf{x}_i^a)), \qquad f \sim GP(\mu, k)$$

where $\Psi(\cdot)$ is a non-negative valued function taken to be $f^2$ or $\exp(f)$. Some features of Gaussian process here:

- Bayesian non-parametric model, i.e. flexible model
- Provides uncertainty on predictions
- Intractable posterior
- Complexity $O(n^3)$

**Main contribution**

For scalable inference, we derived a scheme based on variational inference, with new proposed bounds and approximations.

# Poisson Bag Model

$$y^a|\mathbf{x}^a \sim \text{Poisson}\left(\sum_{i=1}^{N_a} p_i^a \lambda_i^a\right), \qquad \lambda_i^a = \Psi(f(x_i^a)), \qquad f \sim GP(\mu, k)$$

Nonnegative link functions: $\Psi(f) = f^2$ and $\Psi(f) = e^f$.
Standard variational bound using inducing points $u = [f(w_1), \ldots, f(w_m)]^\top$ and a multivariate normal variational posterior $q(u)$

$$\begin{aligned}
\log p(y|\Theta) &= \log \int\int p(y, f, u|X, W, \Theta) df du \\
&\geq \int\int \log\Big\{p(y|f, \Theta)\frac{p(u)}{q(u)}\Big\} p(f|u, \Theta) q(u) df du \quad \text{(Jensen's inequality)} \\
&= \sum_a y^a \int \log\Big(\sum_{i=1}^{N_a} p_i^a \Psi(f(x_i^a)\Big) q(f) df - \sum_a \sum_{i=1}^{N_a} \int p_i^a \Psi(f(x_i^a)) q(f) df \\
&\quad - \sum_a \log(y^a!) - KL(q(u)||p(u)) =: \mathcal{L}(q, \Theta),
\end{aligned}$$

is still intractable due to aggregation. Needs a further lower bound or an approximation.

# Log-sum Lemma

## Lemma

*Let* $v = [v_1, \ldots, v_N]^\top$ *be a random vector with probability density* $q(v)$*, and let* $w_i \geq 0$*,* $i = 1, \ldots, N$*. Then, for any non-negative valued function* $\Psi(v)$*,*

$$\int \log\Big(\sum_{i=1}^{N} w_i \Psi(v_i)\Big) q(v) dv \geq \log\Big(\sum_{i=1}^{N} w_i e^{\xi_i}\Big),$$

*where*

$$\xi_i := \int \log \Psi(v_i) q_i(v_i) dv_i.$$

Additionally, a Taylor approximation can be used for $\Psi(f) = f^2$ (where intractable term essentially becomes $\mathbb{E} \log \|V\|^2$ where $V$ is a multivariate normal) – note that log-sum lemma still gives a lower bound in terms of special functions in that case (problematic for backpropagation!)

# Inference

For scalability and tractability, we use variational inference [2] with approximating distribution $q(u) \sim \mathcal{N}(\eta_u, \Sigma_u)$. This leads us to:

1. $\Psi(f) = f^2$, an additional approximation using Taylor expansion is applied.

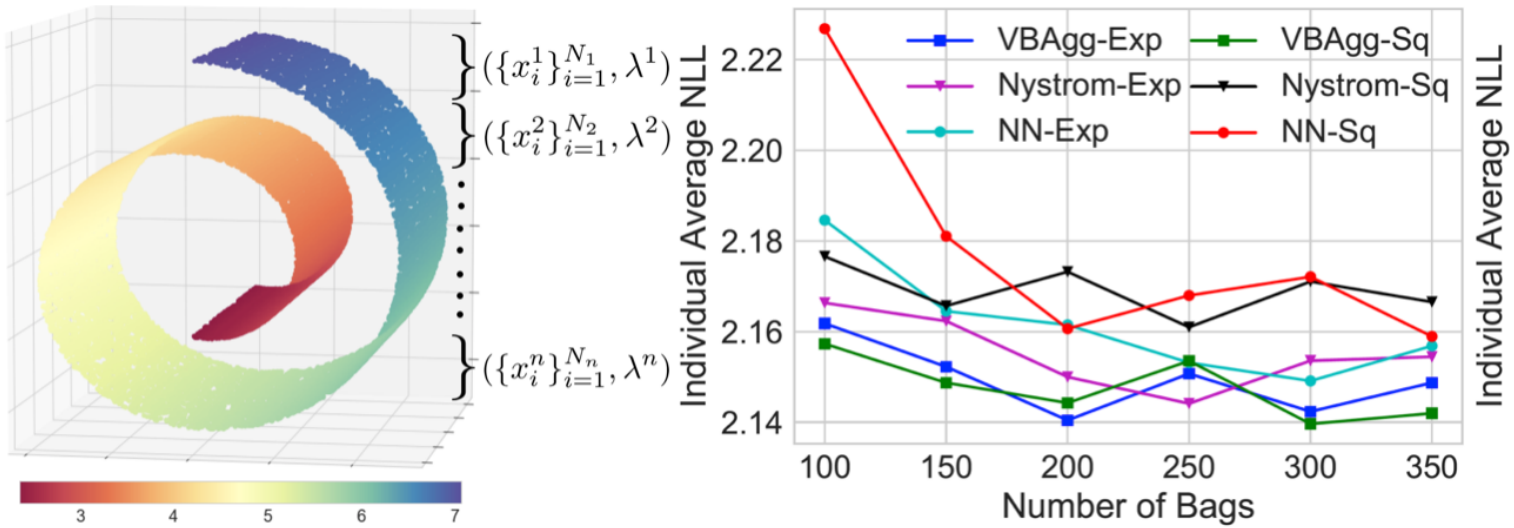
$$\mathcal{L}_1^s := \sum_{a=1}^{n} y^a \zeta^a - \sum_{a=1}^{n} \sum_{i=1}^{N_a} \left\{ (m_i^a)^2 + S_{ii}^a/2 \right\} - KL(q(u)||p(u|W))$$

2. $\Psi(f) = \exp(f)$, an additional lower bound is taken.

$$\mathcal{L}_1^e := \sum_{a=1}^{n} y^a \log\left(\sum_{i=1}^{N_a} e^{m_i^a}\right) - \sum_{j=1}^{n} \sum_{i=1}^{N_a} e^{m_i^a + S_{ii}^a/2} - KL(q(u)||p(u|W)).$$

We can optimise these w.r.t variational parameters $\{\eta_u, \Sigma_u\}$, kernel parameters, using stochastic gradient descent (SGD).

# Toy experiment




**Goal:** Predict the underlying incidence rate (represented by the colour)
**Data:** Simulated data, where covariates $\mathbf{x}_i^a$ are locations on the swiss roll, and bags are constructed through moving along the $z$-axis.

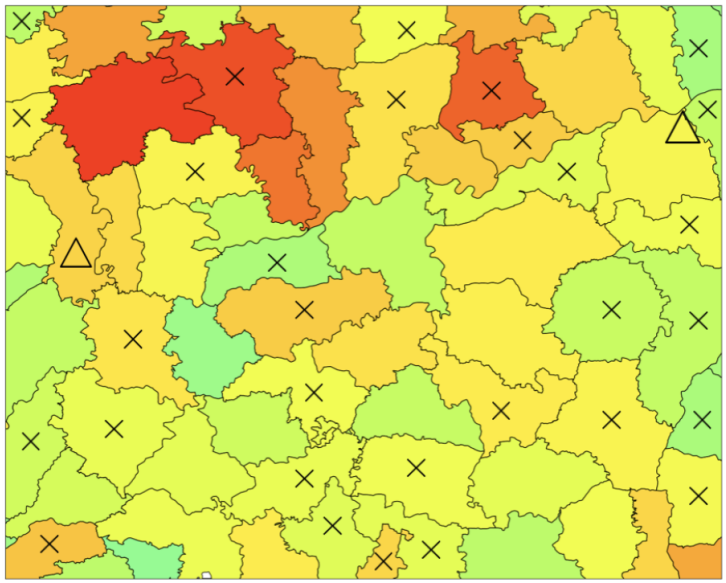
Tensorflow implementation: https://github.com/hcllaw/VBAgg

# Results on Malaria data

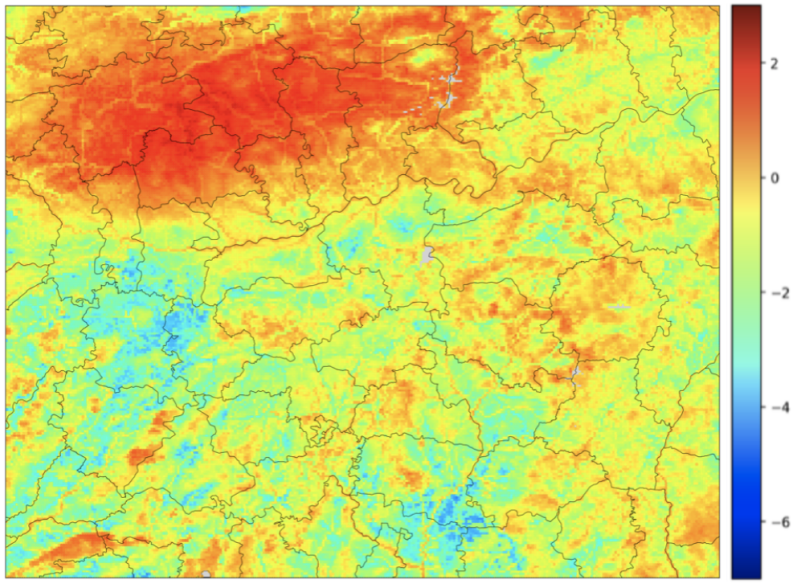
**Goal:** Predict the underlying malaria incidence rate in each 1km by 1km region (pixel)

**Data:** Aggregated incidence of malaria $y^a$ at $957$ regions, where $N_a$ ranges from $13$ to $6,667$, with a total of $1,044,683$ pixels. Covariates $\mathbf{x}_i^a \in \mathbb{R}^{18}$, collected by remote sensing.

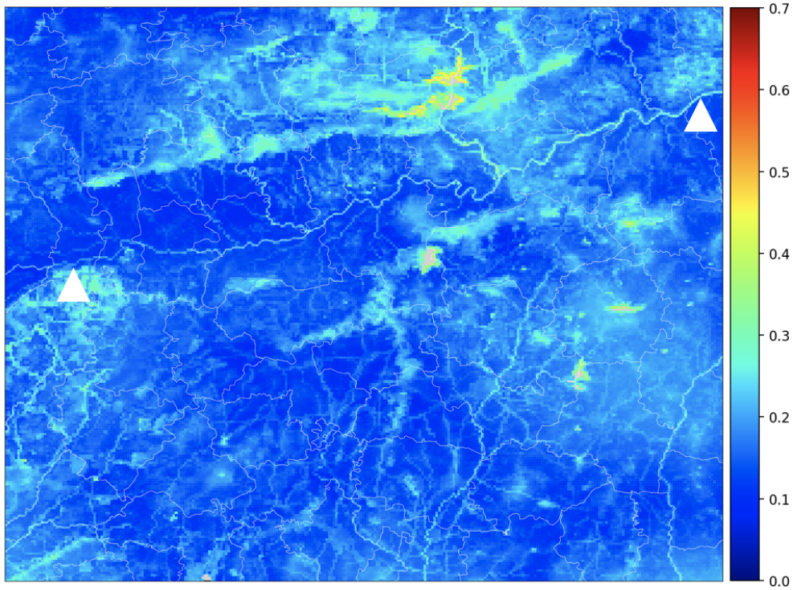
# Malaria results



Data (constant)




Predicted




Uncertainty

- Log incidence rate of malaria per 1000.
- Triangle denotes approximate start and end of river location, a widely reported association with malaria.
- Crosses denotes non-train set bags.

# Summary

- Learning on aggregates: the responses are only available at the coarse level. Statistical modelling can be brought to bear in tandem with performant machine learning models.
- Increasing confluence between statistics and ML: making use of the well engineered (deep) learning infrastructure, while carefully considering appropriate statistical models for the problem at hand.
- Flexibility of the RKHS framework and Gaussian processes as a common ground between machine learning and statistical inference.

# Reference

- Ho Chung Leon Law, DS, Ewan Cameron, Tim Lucas, Seth Flaxman, Katherine Battle, and Kenji Fukumizu, Variational Learning on Aggregate Outputs with Gaussian Processes, in *Advances in Neural Information Processing Systems (NeurIPS)*, 2018. *ArXiv e-prints:1805.08463*, 2018.