Beyond mean modelling: multi-parameter GAMs

Matteo Fasiolo

matteo.fasiolo@bristol.ac.uk

Material available at:

`https://github.com/mfasiolo/GAM_Workshop_Enbis_EDF_23`

These slides cover:

1. Multi-parameter GAMs and GAMLSSs
2. Multivariate Gaussian GAMs
3. Stacking and aggregation of experts

Recall GAM model structure:

$$y|\boldsymbol{x} \sim \text{Distr}\{y|\theta_1 = \mu(\boldsymbol{x}), \theta_2, \dots, \theta_p\},$$

where

$$g\{\mu(\boldsymbol{x})\} = \sum_{j=1}^{m} f_j(\boldsymbol{x}).$$

Multi-parameter GAM structure (Wood et al., 2016):

$$y|\boldsymbol{x} \sim \text{Distr}\{y|\theta_1 = \mu_1(\boldsymbol{x}), \theta_2 = \mu_2(\boldsymbol{x}), \dots, \theta_p = \mu_p(\boldsymbol{x})\},$$

where

$$g_1\{\mu_1(\boldsymbol{x})\} = \sum_{j=1}^{m} f_j^1(\boldsymbol{x}), \quad \dots \quad g_p\{\mu_p(\boldsymbol{x})\} = \sum_{j=1}^{m} f_j^p(\boldsymbol{x}).$$

The role of $\theta_1, \dots \theta_p$ determines the type of model.

Special case are **Generalized Additive Models for Location Scale and Shape** (GAMLSS) (Rigby and Stasinopoulos, 2005).

Example: **Gaussian location-scale model**

Model is

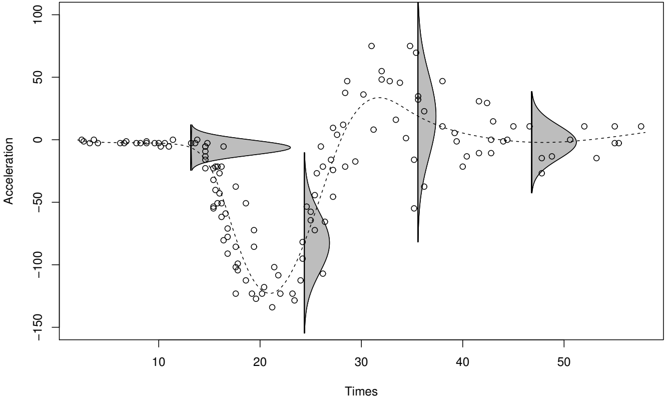
$$y|\boldsymbol{x} \sim N\{y|\mu(\boldsymbol{x}), \sigma^2(\boldsymbol{x})\}$$

where

$$\mu(\boldsymbol{x}) = \sum_{j=1}^{m} f_j^1(\boldsymbol{x})$$

$$\log \sigma(\boldsymbol{x}) = \sum_{j=1}^{m} f_j^2(\boldsymbol{x})$$

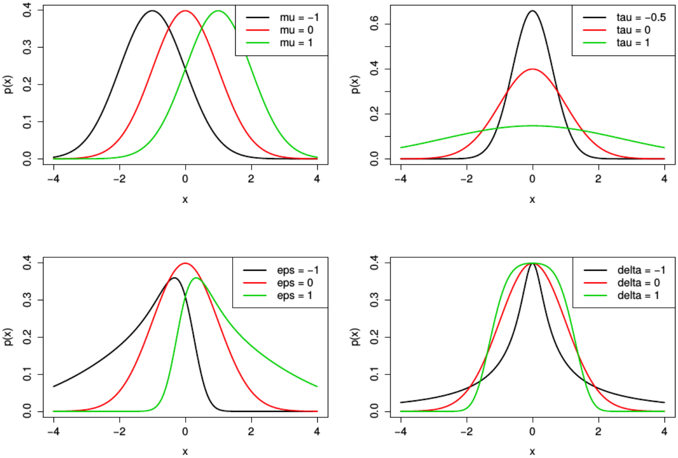
See appendix for complete list of distributions in `mgcv`.

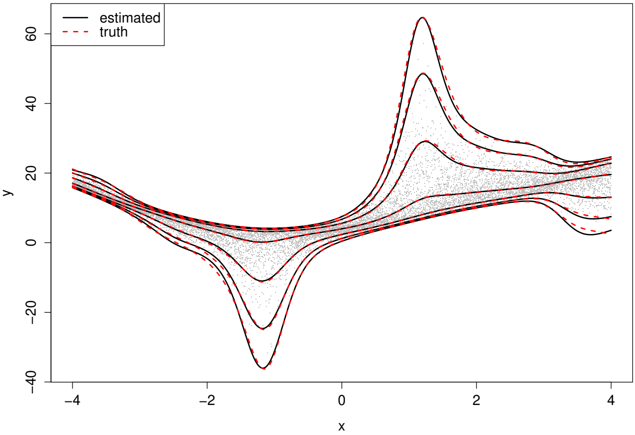


In mgcv: `gam(list(y ~ s(x), ~ s(x)), family=gaulss)`.

Example: **Sinh-arcsinh (shash) distribution**

Four parameter distribution where location, scale, skewness (asymmetry) and kurtosis (tail behaviour) can depend on **x** (Jones and Pewsey, 2009).





`gam(list(y~s(x), ~s(x), ~s(x), ~s(x)), family=shash).`

Let's look at R_demos/3_multi_gams.html

These slides cover:

1. Multi-parameter GAMs and GAMLSSs
2. Multivariate Gaussian GAMs
3. Stacking and aggregation of experts

Non-GAMLSS example: **multivariate normal GAMs**

$$\boldsymbol{y} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_d \end{pmatrix} \sim \mathrm{N}\left(\begin{pmatrix} \mu_1(\boldsymbol{x}) \\ \mu_2(\boldsymbol{x}) \\ \mu_3(\boldsymbol{x}) \\ \vdots \\ \mu_d(\boldsymbol{x}) \end{pmatrix}, \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \cdots & \cdots & \Sigma_{1d} \\ \Sigma_{12} & \Sigma_{22} & \cdots & \cdots & \Sigma_{2d} \\ \Sigma_{13} & \Sigma_{23} & \cdots & \cdots & \Sigma_{3d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \Sigma_{1d} & \Sigma_{2d} & \cdots & \cdots & \Sigma_{dd} \end{pmatrix} \right).$$

In `mgcv` you can do:

```
fit <- gam(list(y1 ~ s(x1),
                y2 ~ s(x3),
                y3 ~ s(x3)),
           family = mvn(3))
```

With the `SCM` package we can model $\boldsymbol{\Sigma}$ as well

$$\boldsymbol{y} \sim N(\boldsymbol{\mu}(\boldsymbol{x}), \boldsymbol{\Sigma}(\boldsymbol{x})).$$

$\boldsymbol{\Sigma}(\boldsymbol{x})$ must be positive definite so we can **not** write $\Sigma_{jk} = \sum_j f_j(\boldsymbol{x})$.

One option is the modified Cholesky decomposition (Pourahmadi, 1999)

$$\boldsymbol{\Sigma}^{-1} = \boldsymbol{T}^{\top} \boldsymbol{D}^{-2} \boldsymbol{T}\,,$$

where $\boldsymbol{D}^2$ is a diagonal matrix and $\boldsymbol{T}$ is upper triangular.

Why the MCD?

If $\boldsymbol{r} = \boldsymbol{y} - \boldsymbol{\mu}$ then $\text{cov}(\boldsymbol{r}) = \boldsymbol{\Sigma}$ and $\boldsymbol{\Sigma}^{-1} = \boldsymbol{T}^\top \boldsymbol{D}^{-2} \boldsymbol{T}$.

Consider simulated residuals s.t. $\text{var}(\tilde{r}_1) = D^2_{1,1}$ and

$$\tilde{r}_l = -\sum_{k=1}^{l-1} T_{l,k} \tilde{r}_k + \epsilon_l \ , \quad \text{var}(\epsilon_l) = \mathrm{D}^2_{l,l} \, ,$$

where

$$\boldsymbol{T} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ T_{2,1} & 1 & 0 & \cdots & 0 \\ T_{3,1} & T_{3,2} & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ T_{14,1} & T_{14,2} & \cdots & T_{14,13} & 1 \end{pmatrix},$$

then $\text{cov}(\tilde{\boldsymbol{r}}) = \boldsymbol{\Sigma}$.

Available via the `SCM` package (Gioia et al., 2025):

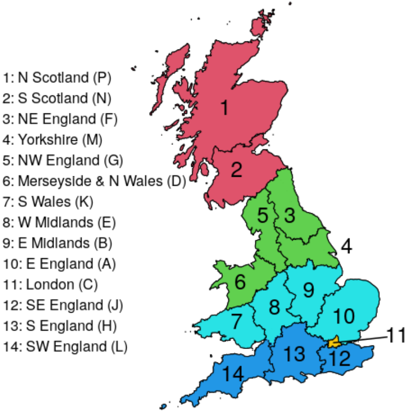
`https://github.com/VinGioia90/SCM`:

To install type:

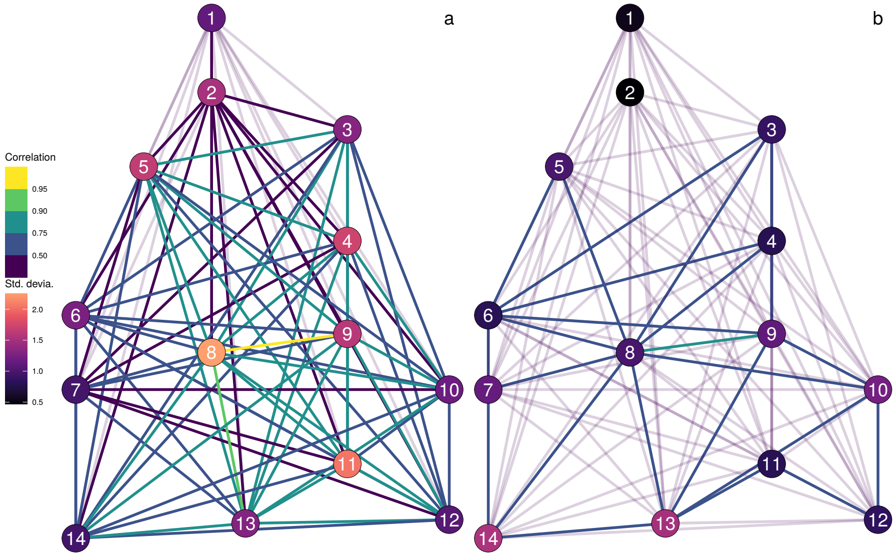
```
library(devtools)
install_github("VinGioia90/SCM")
```

See Gioia et al. (2024) for details.

The UK electricity grid is divided into 14 grid supply groups (GSP).



Gioia et al. (2024) produce **joint** probabilistic forecasts of net-demand.



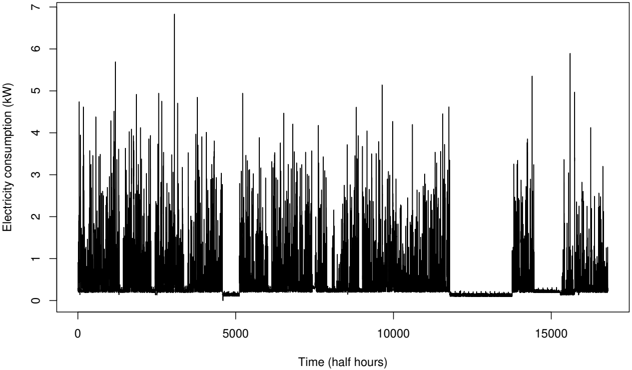
Left: 7am 31/12/2018. Right: midnight 20/08/2018.

Now continue example on `3_multi_gams.html`.

These slides cover:

1. Multi-parameter GAMs and GAMLSSs
2. Multivariate Gaussian GAMs
3. Stacking and aggregation of experts

Non-GAMLSS example: **additive stacking** or **aggregation of experts**



Two models for log-demand at time t or day d:

1. $\log \text{dem}_{td} \sim N(\mu = f(\text{time\_of\_day}_t), \sigma^2)$
2. $\log \text{dem}_{td} \sim N(\mu = \text{mean}(\log \mathbf{dem}_{d-1}), \sigma^2 = \text{var}(\log \mathbf{dem}_{d-1}))$

where $\mathbf{dem}_d = \{\log \text{dem}_{1d}, \dots, \log \text{dem}_{48d}\}$.

We want to predict $y|\boldsymbol{x}$ and we have models $p_1(y|\boldsymbol{x}), \dots, p_K(y|\boldsymbol{x})$.

Build mixture with covariate-dependent weights

$$p_{\text{mix}}(y|\boldsymbol{x}) = \sum_{k=1}^{K} w_k(\boldsymbol{x}) p_k(y|\boldsymbol{x});$$

where $0 \leq w_k \leq 1$ and $\sum_k w_k = 1$.

Capezza et al. (2021) use the multinomial parametrisation

$$w_k = \frac{e^{\eta_k}}{\sum_j e^{\eta_j}},$$

with $\eta_1 = 0$ and $\eta_k = \sum_l f_{lk}(\boldsymbol{x})$ for $k = 2, \dots, K$.

Available via the `gamFactory`:

```
install_github("mfasiolo/gamFactory")
```

For more advanced methods see `gamstackr` package:

`https://github.com/eenticott/gamstackr`

by Euan Enticott.

Now continue example on `3_multi_gams.html`.

For related approaches see Yao et al. (2022) and Rügamer et al. (2022).

References I

Capezza, C., B. Palumbo, Y. Goude, S. N. Wood, and M. Fasiolo (2021). Additive stacking for disaggregate electricity demand forecasting. *The Annals of Applied Statistics* **15**(2), 727–746.

Gioia, V., M. Fasiolo, R. Bellio, and S. N. Wood (2025). Scalable fitting methods for multivariate gaussian additive models with covariate-dependent covariance matrices. *arXiv preprint arXiv:2504.03368*.

Gioia, V., M. Fasiolo, J. Browell, and R. Bellio (2024). Additive covariance matrix models: Modeling regional electricity net-demand in great britain. *Journal of the American Statistical Association*, 1–13.

Jones, M. and A. Pewsey (2009). Sinh-arcsinh distributions. *Biometrika 96*(4), 761–780.

Pourahmadi, M. (1999). Joint mean-covariance models with applications to longitudinal data: Unconstrained parameterisation. *Biometrika* **86**(3), 677–690.

Rigby, R. A. and D. M. Stasinopoulos (2005). Generalized additive models for location, scale and shape. *Journal of the Royal Statistical Society: Series C (Applied Statistics) 54*(3), 507–554.

References II

Rügamer, D., F. Pfisterer, B. Bischl, and B. Grün (2022). Mixture of experts distributional regression: Implementation using robust estimation with adaptive first-order methods. *arXiv preprint arXiv:2211.09875*.

Wood, S. N., N. Pya, and B. Säfken (2016). Smoothing parameter and model selection for general smooth models. *Journal of the American Statistical Association 111*(516), 1548–1575.

Yao, Y., G. Pirš, A. Vehtari, and A. Gelman (2022). Bayesian hierarchical stacking: Some models are (somewhere) useful. *Bayesian Analysis 17*(4), 1043–1071.

List of distributions in mgcv

Type `?mgvc::family` on the R console to see a list of distributions from the exponential family.

Wood et al. (2016) allows Distr $\notin$ exponential family (**extended GAMs**):

1. `scat` $\rightarrow$ scaled Student-t;
2. `betar` $\rightarrow$ beta for $y \in (0, 1)$;
3. `ziP` $\rightarrow$ zero-inflated Poisson;
4. `tw` $\rightarrow$ Tweedie;
5. `ocat` $\rightarrow$ order categorical;
6. `nb` $\rightarrow$ negative binomial.

Note that these EGAMs have one linear predictor, i.e.

$$y_i | \boldsymbol{x}_i \sim \text{Distr}\{y_i | \theta_1(\boldsymbol{x}), \theta_2, \dots, \theta_p\}.$$

hence are not GAMLSSs.

Available GAMLSS families:

1. `gammals` $\rightarrow$ 2-par gamma;
2. `gaulss` $\rightarrow$ 2-par Gaussian;
3. `shash` $\rightarrow$ 4-par sinh-arsinh;
4. `ziplss` $\rightarrow$ 2-par zero-inflated Poisson;
5. `gevlss` $\rightarrow$ 3-par generalised extreme value distribution (GEV);
6. `gumbls` $\rightarrow$ 2-par Gumbel (special case of GEV);
7. `twlss` $\rightarrow$ 3-par Tweedie.

Further models are:

1. `multinom` $\rightarrow$ multinomial categorical;
2. `cox.ph` $\rightarrow$ Cox Proportional Hazards model;
3. `mvn` $\rightarrow$ multivariate Gaussian model (fixed covariance).