# Orthogonal Bases for Multi-Output Gaussian Processes

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# Contents

# Introduction

# Gaussian Processes

- A powerful and popular probabilistic modelling framework for nonlinear functions.
- Definition: $f \sim \mathcal{GP}(m, k)$ if, for all $(t_1, \ldots, t_n) \in \mathcal{T}^n$,

$$\begin{bmatrix} f(t_1) \\ \vdots \\ f(t_n) \end{bmatrix} \sim \mathcal{N}\left( \begin{bmatrix} m(t_1) \\ \vdots \\ m(t_n) \end{bmatrix}, \begin{bmatrix} k(t_1, t_1) & \cdots & k(t_1, t_n) \\ \vdots & \ddots & \vdots \\ k(t_n, t_1) & \cdots & k(t_n, t_n) \end{bmatrix} \right).$$

- Inference and learning: $O(n^3)$ time and $O(n^2)$ memory.

# Multi-Output Gaussian Processes

- Multi-output GPs go long way back (Matheron, 1969).
- Vector-valued mean function $m$ and matrix-valued kernel $K$:

$$m\colon \mathcal{T} \to \mathbb{R}^p, \quad K\colon \underset{\substack{\uparrow \\ \text{input space} \\ \text{(time)}}}{\mathcal{T}^2} \to \mathbb{R}^{p\times p}, \longleftarrow \begin{matrix}\text{number of}\\ \text{outputs}\end{matrix}$$

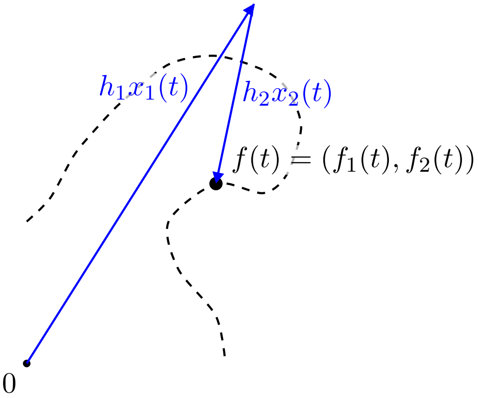
$$m(t) = \begin{bmatrix} \mathbb{E}[f_1(t)] \\ \vdots \\ \mathbb{E}[f_p(t)] \end{bmatrix},$$

$$K(t,t') = \begin{bmatrix} \operatorname{cov}(f_1(t), f_1(t')) & \cdots & \operatorname{cov}(f_1(t), f_p(t')) \\ \vdots & \ddots & \vdots \\ \operatorname{cov}(f_p(t), f_1(t')) & \cdots & \operatorname{cov}(f_p(t), f_p(t')) \end{bmatrix}.$$

- Inference and learning: $O(n^3 p^3)$ time and $O(n^2 p^2)$ memory.
  - Often alleviated by exploiting structure in $K$.

# The Linear Mixing Model

# Fixed Basis with Varying Coefficients



$$f(t) = h_1x_1(t) + h_2x_2(t) = \underbrace{\begin{bmatrix} h_1 & h_2 \end{bmatrix}}_{H} \underbrace{\begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}}_{x(t)}.$$

# The Linear Mixing Model

“mixing matrix”

**Definition (Linear Mixing Model)**

$$x \sim \mathcal{GP}(0, K(t,t')), \quad f(t) \,|\, H, x = Hx(t), \quad y \,|\, f \sim \mathcal{GP}(f(t), \Lambda).$$

“latent processes”

- $f$ is $p$-dimensional, $x$ is $m$-dimensional, and $H$ is $p \times m$.
    - Often $p \gg m$.
- Equivalently, $y \sim \mathcal{GP}(0, HK(t,t')H^\mathsf{T} + \Lambda)$.
- Generalisation of FA to time series setting.
- Fixed spatial correlation: $\mathbb{E}[f(t)f^\mathsf{T}(t)] = HH^\mathsf{T}$ if $K(t,t) = I$.
- Instantaneous mixing: $f(t)$ depends on $x(t')$ only for $t = t'$.
- Inference and learning: $O(n^3 m^3)$ time and $O(n^2 m^2)$ memory.

# Exploiting the Low-Rank Structure

### Proposition

Let $T$ be the $(m \times p)$-matrix $(H^\top \Lambda^{-1} H)^{-1} H^\top \Lambda^{-1}$. Then

$$\text{conditioning } y \mid f \sim \mathcal{GP}(f(t), \Lambda) \text{ on data } Y\text{: } O(n^3 p^3)$$

$$\Longleftrightarrow$$

$$\text{conditioning } \underbrace{Ty}_{u} \mid f \sim \mathcal{GP}(\underbrace{Tf(t)}_{x(t)}, T\Lambda T^\top) \text{ on data } TY\text{: } O(n^3 m^3).$$

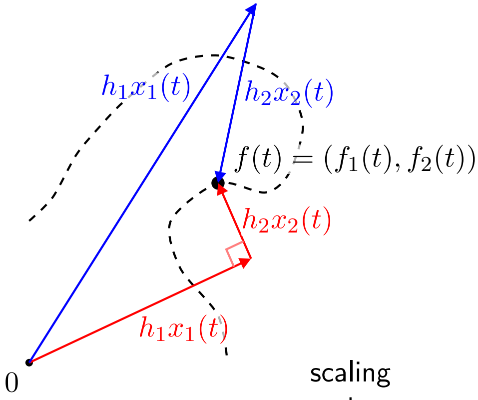
- $T$: "$y$-space" → "$x$-space".
- $Ty = \arg\min_x \|\Lambda^{\frac{1}{2}}(y - Hx)\|_2$.

$$\begin{tikzcd}
Y \arrow[r, "\text{inference}", "O(n^3 p^3)"'] \arrow[d] & p(y \mid Y) \\
TY \arrow[r, "\text{inference}", "O(n^3 m^3)"'] & p(u \mid TY) \arrow[u]
\end{tikzcd}$$

What if $T\Lambda T^\top$ were diagonal? Then inference decouples into independent problems!

# The Orthogonal Linear Mixing Model

# Fixed Orthogonal Basis with Varying Coefficients



$$\begin{bmatrix} h_1 & h_2 \end{bmatrix} = H = \underset{\substack{\uparrow \\ \text{orthogonal}}}{U} \overset{\substack{\text{scaling} \\ \downarrow}}{S}^{\frac{1}{2}}.$$

# The Orthogonal Linear Mixing Model

**Definition (Orthogonal Linear Mixing Model)**

With $K(t,t) = I$, $H = US^{\frac{1}{2}}$, and $\Lambda = \sigma^2 I + HDH^{\mathsf{T}}$,

$$x \sim \mathcal{GP}(0, K(t,t')), \quad f(t) \,|\, H, x = Hx(t), \quad y \,|\, f \sim \mathcal{GP}(f(t), \Lambda).$$

- Generalisation of PPCA (Tipping and Bishop, 1999) to time series setting.
- Like GPFA (Yu et al., 2009), but orthogonality built in.
- General spatial correlation: $\mathbb{E}[f(t)f^{\mathsf{T}}(t)] = USU^{\mathsf{T}}$.
  - ⇒ Suggests way to initialise $U$ and $S$.

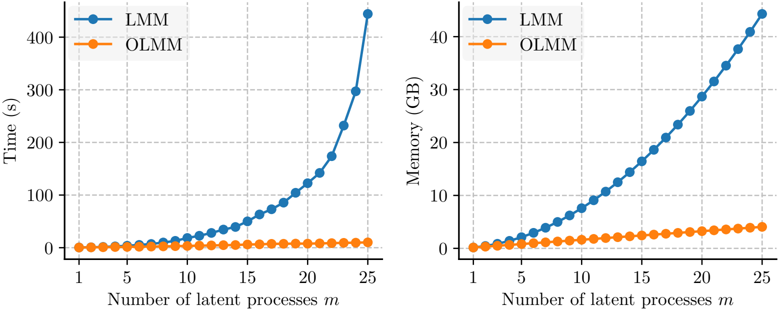
# Inference and Learning

- Image of noise: $T\Lambda T^{\mathsf{T}} = \sigma^2 S^{-1} + D$. Diagonal!

$$\begin{tikzcd}
Y \arrow[r, "\text{inference}", "O(n^3 p^3)"'] \arrow[dd] & p(y \,|\, Y) \\
 & p(u_1 \,|\, (TY)_{1:}) \arrow[u, bend right] \\
TY \arrow[ur, "\text{inference}", "O(n^3)"'] \arrow[dr, "\text{inference}", "O(n^3)"'] & \vdots \\
 & p(u_m \,|\, (TY)_{m:}) \arrow[uuu, bend right]
\end{tikzcd}$$

- Inference and learning: $O(n^3 m)$ time and $O(n^2 m)$ memory.
  $\Rightarrow$ Linear scaling in the number of degrees of freedom!
- Trivially compatible with one-dimensional scaling techniques.

# Inference and Learning (2)



**Proposition**

The evidence $\log p(Y)$ is convex in $U$.

# Arbitrary Likelihoods

# Recapitulation of the OLMM

- \+ Computationally efficient
  - \+ Linear scaling in number of degrees of freedom $m$
  - \+ Trivially compatibly with one-dimensional scaling techniques
  - \+ Convex in $U$
- \+ Easy to implement
- ± Expressivity
  - ± Restricted to orthogonal bases
  - – Linear correlations
- – Cannot handle missing data
- – Cannot handle imhomogeneous observation noise

Goal: arbitrary $p(y \mid f)$ whilst retaining computational efficiency.

# Application: Neural Networks with Time-Varying Weights

Task: predict mapping $z \mapsto \phi(z, t)$ that slowly varies with time.

- ???
- Economics?

Generative model:

$$w \sim \mathrm{OLMM}, \quad \phi(z, t) \,|\, w = \mathrm{NN}_{w(t)}(z).$$

Inference: VI with an OLMM as computationally efficient $q$.

# Variational Inference

Prior:

$$p(y, f) = \underbrace{p(y \,|\, f)}_{\text{arbitrary likelihood}} p(f).$$

Approximate posterior (Johnson et al., 2016):

$$q(f) = \frac{1}{Z} p(f) \underbrace{p(\hat{y} \,|\, f, \hat{\Lambda})}_{\text{likelihood ``conjugate'' to the OLMM}}.$$

ELBO:

$$\mathcal{L}(\hat{y}, \hat{\Lambda}) = \underbrace{\log Z}_{\text{evidence of pseudo-observations}} + \overbrace{\mathbb{E}_{q(f)}[\log p(\underset{\substack{\uparrow \\ \text{tractable / Monte Carlo}}}{y \,|\, f}) - \log p(\underset{\substack{\uparrow \\ \text{tractable}}}{\hat{y} \,|\, f}, \hat{\Lambda})]}^{\text{likelihood correction}}.$$

- \+ Pseudo-evidence $\log Z$ and approximate posterior $q(f)$ cheap
- \+ Easy to implement
- ± Prior $p(f)$ shared with $q(f)$
- − For $k$ pseudo-points, $O(kp)$ parameters

# Variational Inference, Take 2

Approximate posterior:

$$
\begin{aligned}
q(f) &= \frac{1}{Z} p(f) p(\hat{y} \mid f, \hat{\Lambda}) \\
&= \frac{1}{Z} p(f) p(\underbrace{T\hat{y}}_{\hat{u}} \mid f, \underbrace{T\hat{\Lambda}T^{\mathsf{T}}}_{\hat{D}}) = \frac{1}{Z} p(f) p(\hat{u} \mid f, \hat{D}).
\end{aligned}
$$

ELBO:

$$\mathcal{L}(\hat{u}, \hat{D}) = \log Z + \mathbb{E}_{q(f)}[\log p(y \mid f) - \log p(\hat{u} \mid f, \hat{D})].$$

\+ For $k$ pseudo-points, $O(km)$ parameters

# Naturally Mean Field

- $q(f) \propto p(f)p(\hat{u} \,|\, f, \hat{D})$: EP-style approximation in VI setting.
- Consider traditional pseudo-point method (Titsias, 2009):

$$\begin{aligned} q(f) &= \int p(f \,|\, \hat{f}) q(\hat{f}) \, \mathrm{d}\hat{f} \\ &= \int p(f \,|\, \underbrace{T\hat{f}}_{\hat{x}}) q(T\hat{f}) \, \mathrm{d}T\hat{f} = \int p(f \,|\, \hat{x}) q(\hat{x}) \, \mathrm{d}\hat{x}. \end{aligned}$$

- Equivalent if $q(\hat{x}_i) = \mathcal{N}(\hat{u}_i, (K_{x_i}^{-1} + \hat{D}_i^{-1})^{-1})$.
- When does $q^*(\hat{x})$ factorise over the latent processes?

$$\prod_{i=1}^{m} q^*(\hat{x}_i) \overset{?}{=} q^*(\hat{x}) = e^{-\mathcal{L}^*} p(\hat{x}) \exp\langle \log p(y \,|\, x) \rangle_{p(x \,|\, \hat{x})}.$$

① OLMM!
② $y \,|\, x \sim \mathcal{GP}(H\phi(x(t)), \Lambda)$ with $\phi$ a pointwise nonlinearity.

# (Preliminary) Conclusions

# (Preliminary) Conclusions

- Orthogonal basis decouples inference into independent problems.
- OLMM can (maybe) function as a computationally efficient prior / approximate posterior in larger spatio–temporal models.

- Experiments on real-world data!

# Outstanding Questions

- Fixing a computational budget, how does OLMM compare?
- How restrictive is the orthogonality assumption?
  - For a given LMM, how close is the closest OLMM?
- When is $H$ identifiable? Connection to ICA?
- How does learned basis compare to other methods, e.g. PCA?
  - Can pointwise nonlinearity $\phi$ improve learned basis?
- Can orthogonality alleviate downsides of mean-field VI?

These slides: `https://wesselb.github.io/pdf/olmm`.

# Appendix

# References

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