University of Antwerp
Faculty of Applied Engineering

# Constraints on GP Predictions

## Not so normal after all

dr. Ivan De Boi

8 September 2025

# InViLab

## Camera system development

Automation

Prototype development

Camera integration

## Advanced camera technologies

- UV → LWIR
- Multi- and hyperspectral
- 3D imaging
- Variable focus, zoom
- Image intensifiers
- Polarization camera’s

## Camera calibration and fusion

## Image processing and camera simulation

Machine learning

Camera simulation

# 1. The problem with vanilla GPs

# The problem with vanilla GPs

The posterior is a GP!!!

# The problem with vanilla GPs

The posterior is a GP!!!

**Problem locally**: A prediction at $\mathbf{x}$ is a Gaussian distribution, ranging from $1$ to $+1$. What about velocities, weights, heights, concentrations in %, ... ?

# The problem with vanilla GPs

The posterior is a GP!!!

**Problem locally**: A prediction at $\mathbf{x}$ is a Gaussian distribution, ranging from *1* to + *1* . What about velocities, weights, heights, concentrations in %, ... ?

**Problem globally**: Kernel determines shape of the functions. Samples from posterior don't automatically obey monotonicity, convexity, boundary conditions, di erential equations (heat, forces, ...), ...

# The problem with vanilla GPs

The posterior is a GP!!!

**Problem locally**: A prediction at $\mathbf{x}$ is a Gaussian distribution, ranging from $1$ to $+1$. What about velocities, weights, heights, concentrations in %, ... ?

**Problem globally**: Kernel determines shape of the functions. Samples from posterior don't automatically obey monotonicity, convexity, boundary conditions, di erential equations (heat, forces, ...), ...

**Problem multi-output**: Relationships between outputs are not built-in. What about zero curl or divergence in a vector eld? What about unit norm vectors?

# The problem with vanilla GPs

The posterior is a GP!!!

**Problem locally**: A prediction at $\mathbf{x}$ is a Gaussian distribution, ranging from $1$ to $+1$. What about velocities, weights, heights, concentrations in %, ... ?

**Problem globally**: Kernel determines shape of the functions. Samples from posterior don't automatically obey monotonicity, convexity, boundary conditions, di erential equations (heat, forces, ...), ...

**Problem multi-output**: Relationships between outputs are not built-in. What about zero curl or divergence in a vector eld? What about unit norm vectors?

What about your data? **Does it matter**?

# 2. Problem Locally - Bound Constraints

## Bound Constraints

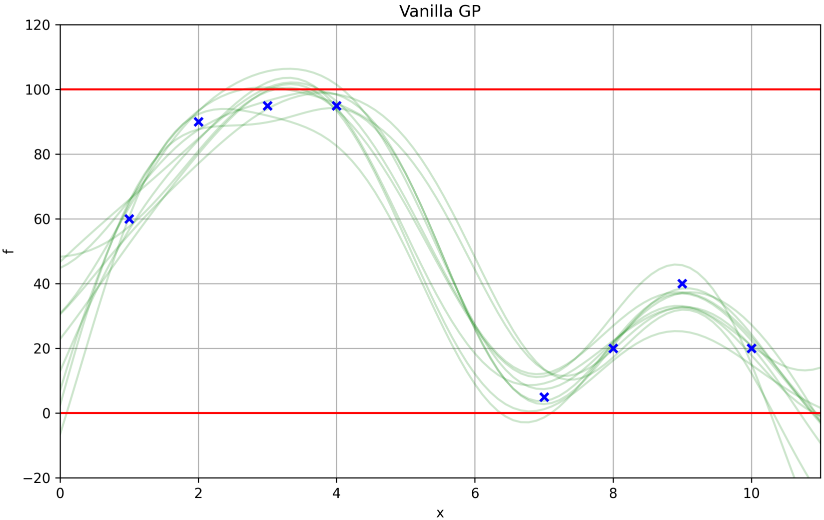
$$a \qquad f(x) \qquad b$$

# Bound Constraints

$$0 \qquad f(x) \qquad 100$$

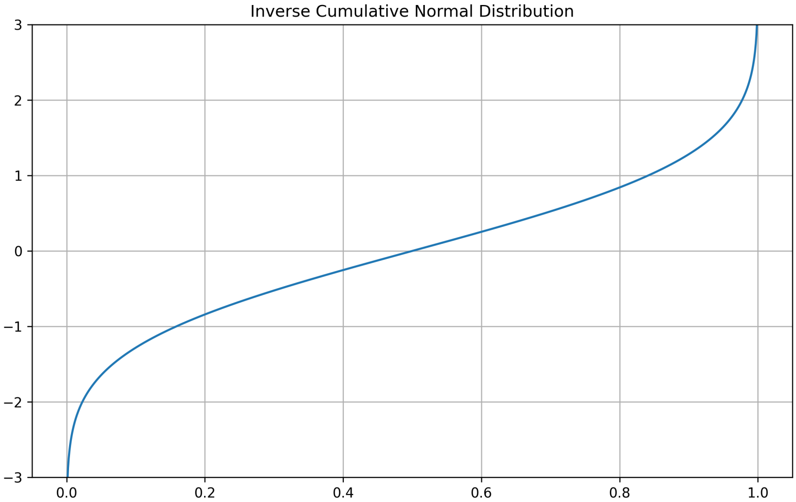
# Bound Constraints

$$0 \qquad f(x) \qquad 100$$



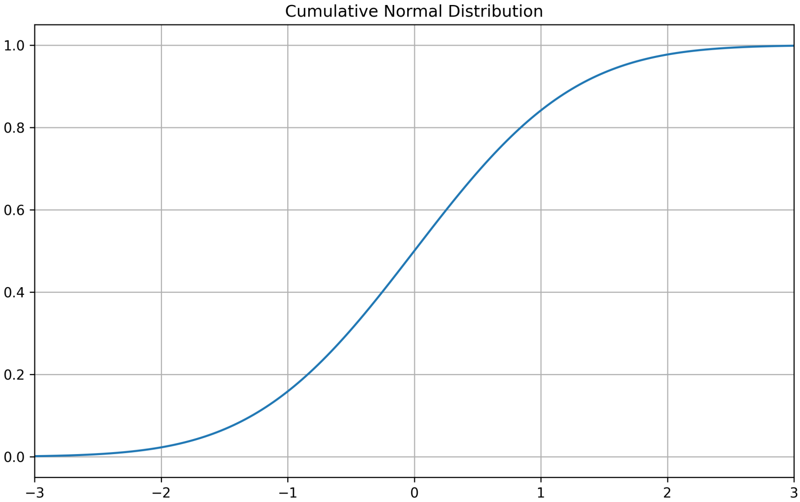
# Bound Constraints - Warping

$$0 \leq f(x) \leq 100, \; u_i = \Phi^{-1}(y_i), \; [0;1] \rightarrow [-\infty; +\infty]$$



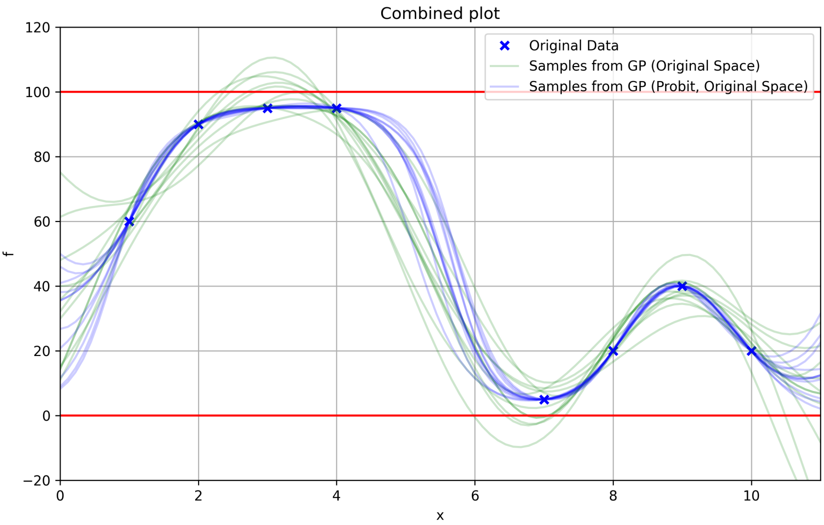
# Bound Constraints - Warping

train GP on $\{x_i, u_i\}$, warp prediction back via



# Bound Constraints - Warping

$$0 \quad f(x) \quad 100$$



# Bound Constraints - Likelihood Tinkering

$$p(\mathbf{f}|X,y,\ ) = \frac{p(y|X,\mathbf{f},\ )p(\mathbf{f}|X,\ )}{p(y|X,\ )}$$

# 3. Problem Globally - Differential Equation Constraints

# Differential Equation Constraints with Data

$Lu = f$, with data on $u$ and $f$, and $L$ linear partial di erential operator

$$u \sim GP(m(\mathbf{x}); k(\mathbf{x}; \mathbf{x}'))$$

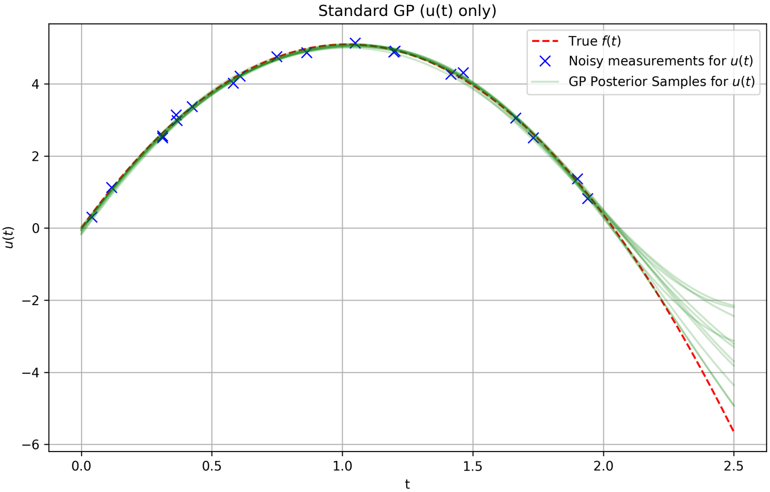
$$Lu \sim GP(L_{\mathbf{x}} m(\mathbf{x}); L_{\mathbf{x}} L_{\mathbf{x}'} k(\mathbf{x}; \mathbf{x}'))$$

$$\begin{bmatrix} u(X_1) \\ f(X_2) \end{bmatrix} \sim GP\left( \begin{bmatrix} m(X_1) \\ Lm(X_2) \end{bmatrix} ; \begin{bmatrix} K_{11}(X_1; X_1) & K_{12}(X_1; X_2) \\ K_{21}(X_2; X_1) & K_{22}(X_2; X_2) \end{bmatrix} \right)$$

$$k\left( \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix} ; \begin{bmatrix} \mathbf{x}_1' \\ \mathbf{x}_2' \end{bmatrix} \right) = \begin{bmatrix} k(\mathbf{x}_1; \mathbf{x}_1') & L_{\mathbf{x}'} k(\mathbf{x}_1; \mathbf{x}_2') \\ L_{\mathbf{x}} k(\mathbf{x}_2; \mathbf{x}_1') & L_{\mathbf{x}} L_{\mathbf{x}'} k(\mathbf{x}_2; \mathbf{x}_2') \end{bmatrix} = \begin{bmatrix} K_{11} & K_{12} \\ K_{21} & K_{22} \end{bmatrix}$$

# Differential Equation Constraints with Data

Kick a ball: height $u(t) = at \quad \frac{g}{2}t^2$ for some unknown $a$.
We observe $u_i$.

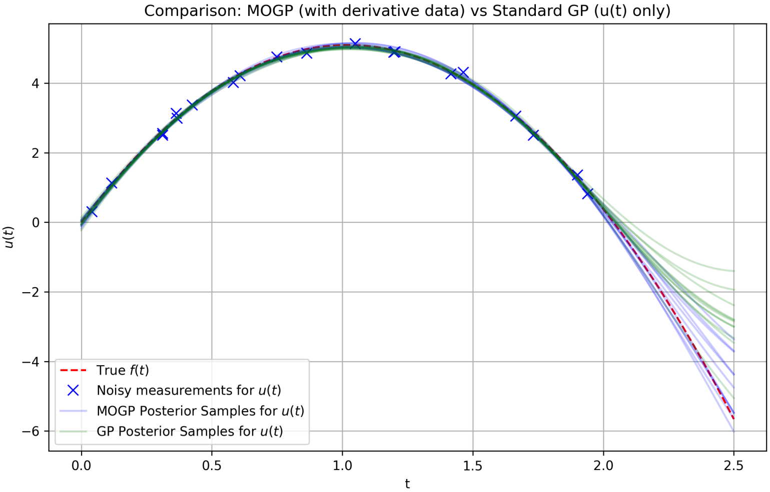



University of Antwerp
Faculty of Applied Engineering

# Differential Equation Constraints with Data

Kick a ball: height $u(t) = at \quad \frac{g}{2}t^2$ for some unknown $a$.

We observe $u_i$ and know $f(t) = \frac{d^2u}{dt^2} = \quad g = f_i$.

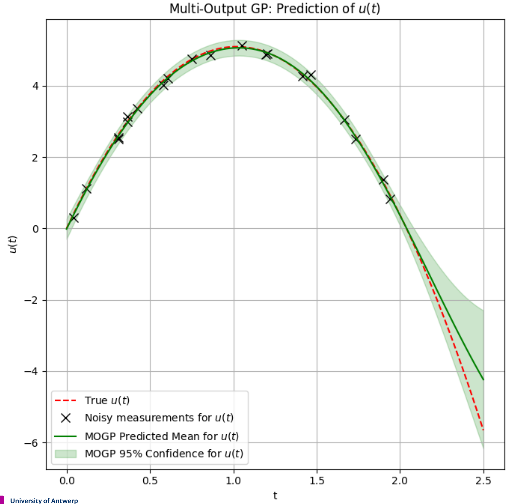


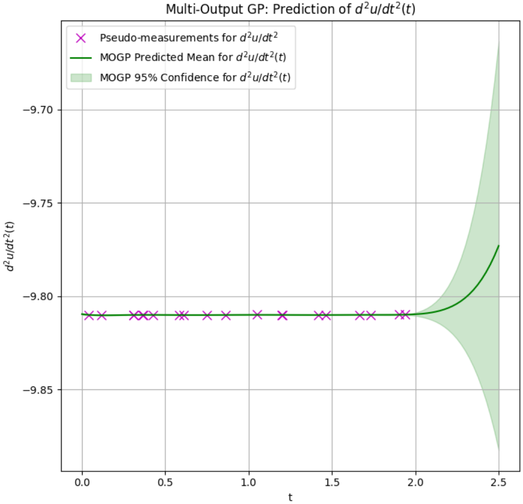

University of Antwerp | Faculty of Applied Engineering

# Differential Equation Constraints with Data

Kick a ball: height $u(t) = at \quad \frac{g}{2}t^2$ for some unknown $a$.

We observe $u_i$ and know $f(t) = \frac{d^2u}{dt^2} = \quad g = f_i$.



# Monotonicity Constraint

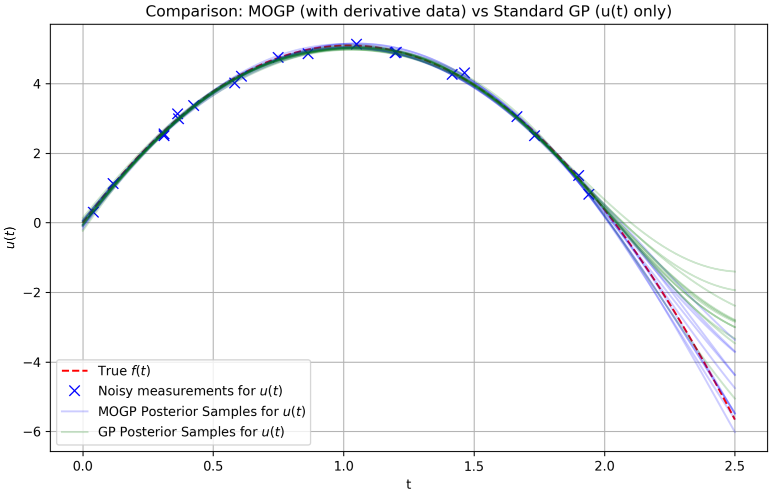
$$\frac{df}{dt} > 0$$

# Convexity Constraint

$$\frac{d^2f}{dt^2} > 0$$

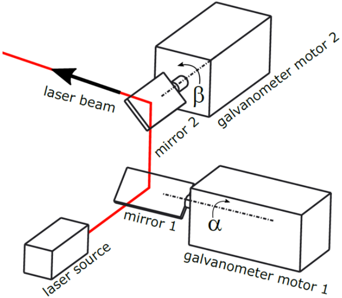
# Concavity Constraint

$$\frac{d^2 f}{dt^2} < 0$$

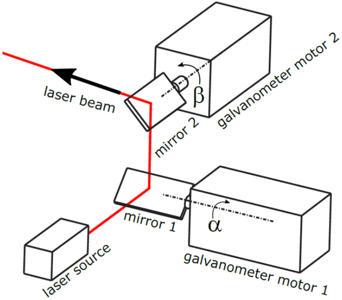


# 4. Problem Multi-Output - e.g. Predict Lines in 3D

# Galvanometric Laser Scanner

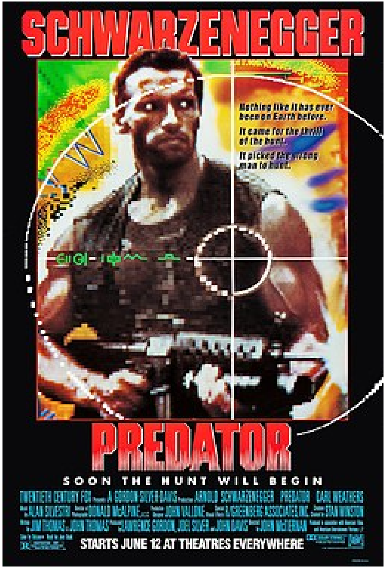



# Galvanometric Laser Scanner

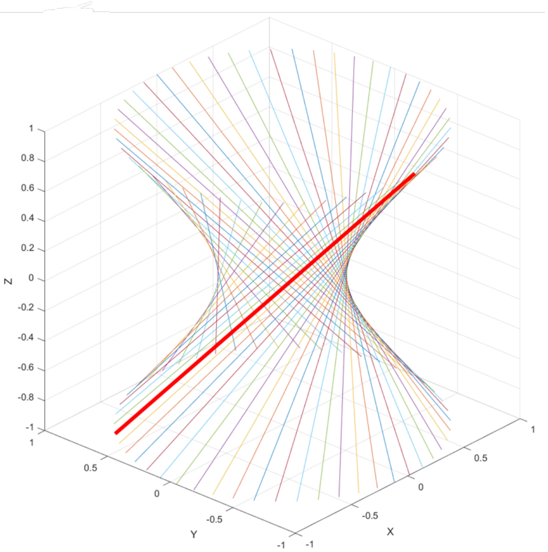



( ; ) ! L

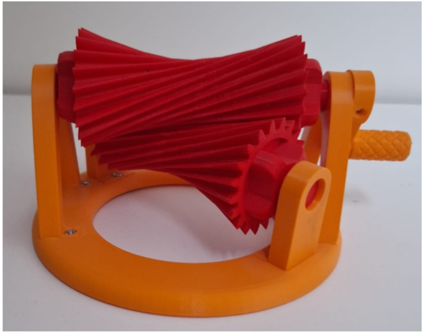
# Predator


SCHWARZENEGGER
Nothing like it has ever been on Earth before.
It came for the thrill of the hunt.
It picked the wrong man to hunt.
PREDATOR
SOON THE HUNT WILL BEGIN
STARTS JUNE 12 AT THEATRES EVERYWHERE

# Hyperboloid



# Hyperboloids


# Hyperboloid Bridge

**Corporation Street Bridge**

| | |
|---|---|
| **Coordinates** | 53°29′01″N 2°14′36″W |
| **Crosses** | Corporation Street |
| **Locale** | Manchester, England |

# Plücker Coordinates

# Plücker Coordinates

$L$ given by moment

$\mathbf{m}$ and direction $\mathbf{d}$ : $(l_1 : l_2 : l_3 : l_4 : l_5 : l_6)$ $2$ $\mathrm{P}^5$

$\mathbf{m}$ $?$ $\mathbf{d}$ $)$ $l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$ (Grassmann-Plücker relationship)

# Plücker Coordinates

$L$ given by moment **m** and direction **d** : $(l_1 : l_2 : l_3 : l_4 : l_5 : l_6)$ 2 $\mathrm{P}^5$

**m** ? **d** ) $l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$ (Grassmann-Plücker relationship)

$L$ 2 $M_2^4$ (Klein Quadric) $\mathrm{P}^5$

# Parallel GPs screw this up

$$(\ ;\ )\ \overset{GP_1}{!}\ l_1$$

$$(\ ;\ )\ \overset{GP_2}{!}\ l_2$$

$$(\ ;\ )\ \overset{GP_3}{!}\ l_3$$

$$(\ ;\ )\ \overset{GP_4}{!}\ l_4$$

$$(\ ;\ )\ \overset{GP_5}{!}\ l_5$$

$$(\ ;\ )\ \overset{GP_6}{!}\ l_6$$

# Parallel GPs screw this up

$$(\quad;\quad)\ \overset{GP_1}{!}\ l_1$$

$$(\quad;\quad)\ \overset{GP_2}{!}\ l_2$$

$$(\quad;\quad)\ \overset{GP_3}{!}\ l_3$$

$$(\quad;\quad)\ \overset{GP_4}{!}\ l_4$$

$$(\quad;\quad)\ \overset{GP_5}{!}\ l_5$$

$$(\quad;\quad)\ \overset{GP_6}{!}\ l_6$$

$$l_1 l_4 + l_2 l_5 + l_3 l_6 = ?$$

# Parallel GPs screw this up

$$(\ ;\ ) \xrightarrow{GP_1} l_1$$

$$(\ ;\ ) \xrightarrow{GP_2} l_2$$

$$(\ ;\ ) \xrightarrow{GP_3} l_3$$

$$(\ ;\ ) \xrightarrow{GP_4} l_4$$

$$(\ ;\ ) \xrightarrow{GP_5} l_5$$

$$(\ ;\ ) \xrightarrow{GP_6} l_6$$

$$l_1 l_4 + l_2 l_5 + l_3 l_6 = ?$$

$$l_1 l_4 + l_2 l_5 + l_3 l_6 \neq 0 \Rightarrow (l_1 : l_2 : l_3 : l_4 : l_5 : l_6) \text{ is a screw, } \in M_2^4$$

NOT a line in 3D!!!

# Constraints on predictions for $L$

$$l_1 l_1 + l_2 l_2 + l_3 l_3 = 1$$

$$l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$$

**5. Unit Norm:** $l_1 l_1 + l_2 l_2 + l_3 l_3 = 1$

# Input ( ; )

Periodic kernel in general:

$$k(\mathbf{x};\mathbf{x}') = \ {}^{2}_{f} \exp \quad \frac{2}{\ell^2} \sin^2 \quad \frac{|\mathbf{x} \quad \mathbf{x}'|}{p}$$

Periodic kernel for $\mathbf{x} = ( \ ; \ )$, ARD and period 2 :

$$k_{PER}(\mathbf{x};\mathbf{x}') = \ {}^{2}_{f} \exp \quad \frac{2}{l^2} \sin^2 \frac{| \qquad {}'|}{2} \quad \exp \quad \frac{2}{l^2} \sin^2 \frac{| \qquad {}'|}{2} \ !$$

# Unit Norm for Direction Vector d

( ; ) ! **d** 2 $R^3$

# Unit Norm for Direction Vector d

$( \quad ; \quad ) \to \mathbf{d} \in \mathbb{R}^3$, constraint: $\|\mathbf{d}\| = 1; \mathbf{d} \in \mathbb{S}^2$

# Unit Norm for Direction Vector d

$( \; ; \; ) \to d \in \mathbb{R}^3$, constraint: $\|d\| = 1; d \in S^2$

New kernel for $x = ( \; ; \; ; \; \mathrm{dim})$, with $\mathrm{dim} \in 1; 2; 3$:

$$k_{PER3D}(x; x') = \begin{cases} k_{PER}([\; ; \;]; [\;'; \;']); & \text{for } \mathrm{dim} = \mathrm{dim}' \\ 0 & \text{for } \mathrm{dim} \neq \mathrm{dim}' \end{cases}$$

# Unit Norm for Direction Vector d

$(\ ;\ ) \to \mathbf{d} \in \mathbb{R}^3$, constraint: $\|\mathbf{d}\| = 1$; $\mathbf{d} \in S^2$

New kernel for $x = (\ ;\ ;\ \mathrm{dim})$, with $\mathrm{dim} \in 1; 2; 3$:

$$k_{PER3D}(x; x') = \begin{cases} k_{PER}([\ ;\ ]; [\ ';\ ']); & \text{for dim} = \text{dim}' \\ 0 & \text{for dim} \neq \text{dim}' \end{cases}$$

$$f_1 : x = \cos(\ )\sin(\ );$$

$$f_2 : y = \sin(\ )\sin(\ );$$

$$f_3 : z = \cos(\ )$$

# Unit Norm for Direction Vector d

$( \; ; \; ) \rightarrow \; d \in \mathbb{R}^3$, constraint: $\|d\| = 1 ; d \in S^2$

New kernel for $x = ( \; ; \; ; \; \text{dim})$, with $\text{dim} \in 1; 2; 3$:

$$k_{PER3D}(x; x') = \begin{cases} k_{PER}([\; ; \;]; [\;' ; \;']) ; & \text{for dim} = \text{dim}' \\ 0 & \text{for dim} \neq \text{dim}' \end{cases}$$

$$f_1 : x = \cos(\;) \sin(\;);$$

$$f_2 : y = \sin(\;) \sin(\;);$$

$$f_3 : z = \cos(\;)$$

$$f_1 \quad \frac{\partial f_2}{\partial} + \frac{\partial f_3}{\partial} = 0$$

# Unit Norm for Direction Vector d

$$f_1 \quad \frac{@f_2}{@} + \frac{@f_3}{@} = 0$$

# Unit Norm for Direction Vector d

$$f_1 \quad \frac{@f_2}{@} + \frac{@f_3}{@} = 0\,,\; F_x[f(x)] = \; 0$$

# Unit Norm for Direction Vector d

$$f_1 \quad \frac{\partial f_2}{\partial} + \frac{\partial f_3}{\partial} = 0\,,\ F_x[f(x)] = 0,\ G_x[g(x)] = f(x)$$

# Unit Norm for Direction Vector d

$f_1 \quad \frac{\partial f_2}{\partial} + \frac{\partial f_3}{\partial} = 0\,,\ F_x[f(x)] = 0,\ G_x[g(x)] = f(x),\ F_x[G_x[g(x)]] = 0,$

# Unit Norm for Direction Vector d

$$f_1 \quad \frac{\partial f_2}{\partial} + \frac{\partial f_3}{\partial} = 0\,,\ F_x[f(x)] = 0,\ G_x[g(x)] = f(x),\ F_x[G_x[g(x)]] = 0,$$

$$g(x) \quad GP(\ _g; k_g); \quad f(x) = G_x g(x) \quad GP(G_x\ \ _g; G_x k_g G_{x'}^T)$$

# Unit Norm for Direction Vector d

$$f_1 \quad \frac{@f_2}{@} + \frac{@f_3}{@} = 0, \; F_x[f(x)] = 0, \; G_x[g(x)] = f(x), \; F_x[G_x[g(x)]] = 0,$$

$$g(x) \quad GP\,( \quad _g; k_g); \quad f(x) = G_x g(x) \quad GP\,(G_x \quad _g; G_x k_g G_{x0}^T)$$

$$F_x = \quad 1; \quad \frac{@}{@}; \frac{@}{@}$$

$$G_x = \quad \frac{@}{@}; 1; 0 \quad ^T; \quad F_x G_x = 0$$

$$G_x G_{x0}^T = \begin{bmatrix} \frac{@^2}{@ \, @_0} & \frac{@}{@} & 0 \\ \frac{@}{@_0} & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

# Unit Norm for Direction Vector d

$$x = ( \; ; \; ; \; \mathrm{dim}), \text{ with dim } 2 \; 1; 2; 3$$

$$k_{\mathrm{PER3D}}(x; x^0) = \begin{cases} k_{\mathrm{PER}}([\;;\;]; [\;^0; \;^0]); & \text{for dim} = \text{dim}^0 \\ 0 & \text{for dim} \neq \text{dim}^0 \end{cases}$$

# Unit Norm for Direction Vector d

$$x = (\;\;;\;\;;\;\;\mathrm{dim}),\ \text{with dim } 2\ 1;2;3$$

$$k_{PER3D}(x;x^0) = \begin{cases} k_{PER}([\;\;;\;\;];[\;^0;\;^0]); & \text{for dim} = \text{dim}^0 \\ 0 & \text{for dim} \neq \text{dim}^0 \end{cases}$$

$$k_{COM}(x;x^0) = \;^2_f \exp\left( \frac{2}{l^2} \sin^2 \frac{\;^0}{2} \right)!$$

$$\exp\left( \frac{2}{l^2} \sin^2 \frac{\;^0}{2} \right)$$

$$\exp\left( \frac{(\text{dim} \;\; \text{dim}^0)^2}{\;^2} \right)$$

# Unit Norm for Direction Vector d

$$k_{DIF} = G_x k_{COM} G_{x0}^T = \begin{bmatrix} A & B & 0 \\ C & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} k_{COM};$$

in which, with $\ = \frac{0}{2}$ (for brevity in notation),

$$A = \frac{\sin^2(\ )\cos^2(\ )}{l^4} + \frac{\cos^2(\ )}{l^2} \quad \frac{\sin^2(\ )}{l^2};$$

$$B = \ \frac{2}{l^2}\sin(\ )\cos(\ );$$

$$C = \frac{2}{l^2}\sin(\ )\cos(\ )$$

# Unit Norm for Direction Vector d

$$k_{DIF} = G_x k_{COM} G_{x_0}^T = \begin{bmatrix} A & B & 0 \\ C & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} k_{COM};$$

in which, with $\quad = \frac{\ \ {}_0}{\ ^2}$ (for brevity in notation),

$$A = \quad \frac{\sin^2(\quad)\cos^2(\quad)}{l^4} + \frac{\cos^2(\quad)}{l^2} \quad \frac{\sin^2(\quad)}{l^2};$$

$$B = \quad \frac{2}{l^2}\sin(\quad)\cos(\quad);$$

$$C = \frac{2}{l^2}\sin(\quad)\cos(\quad)$$

$$(\ ;\quad)\ !\quad d\ 2\ S^2$$

$$f(x) = G_x g(x) \quad GP\,(G_x \quad {}_g; G_x k_g G_{x_0}^T)$$

6. Grassmann-Plücker Relationship: $l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$

# Linear Constraint in general

A set of training examples $\{y_1, \ldots, y_n\}$ that satisfy the linear constraints $Ay_i = b$ will result in a GP for which the mean prediction $(x)$ also satisfies $A(x) = b$.

# Linear Constraint in general

A set of training examples $\{y_1; \ldots; y_n\}$ that satisfy the linear constraints $Ay_i = b$ will result in a GP for which the mean prediction $(x\ )$ also satisfies $A\ (x\ ) = b$.

$$(x\ ) = m_0(x\ ) + K(x\ ; X)\ K(X; X) + \ {}_n^2 I\ ^{1} (y\ \ m(x))$$

# Quadratic Constraint

m ? d ) $l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$, quadratic in $l_i$, but linear in $l_i l_j$

# Quadratic Constraint

m ? d ) $l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$, quadratic in $l_i$, but linear in $l_i l_j$

Let $z = (l_1; l_2; l_3; l_4; l_5; l_6)$ and $Q = z^T z = \begin{bmatrix} l_1 l_1 & l_1 l_2 & l_1 l_3 & l_1 l_4 & l_1 l_5 & l_1 l_6 \\ l_2 l_1 & l_2 l_2 & l_2 l_3 & l_2 l_4 & l_2 l_5 & l_2 l_6 \\ l_3 l_1 & l_3 l_2 & l_3 l_3 & l_3 l_4 & l_3 l_5 & l_3 l_6 \\ l_4 l_1 & l_4 l_2 & l_4 l_3 & l_4 l_4 & l_4 l_5 & l_4 l_6 \\ l_5 l_1 & l_5 l_2 & l_5 l_3 & l_5 l_4 & l_5 l_5 & l_5 l_6 \\ l_6 l_1 & l_6 l_2 & l_6 l_3 & l_6 l_4 & l_6 l_5 & l_6 l_6 \end{bmatrix}$

# Quadratic Constraint

m ? d ) $l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$, quadratic in $l_i$, but linear in $l_i l_j$

Let $z = (l_1; l_2; l_3; l_4; l_5; l_6)$ and $Q = z^T z = \begin{bmatrix} l_1 l_1 & l_1 l_2 & l_1 l_3 & l_1 l_4 & l_1 l_5 & l_1 l_6 \\ l_2 l_1 & l_2 l_2 & l_2 l_3 & l_2 l_4 & l_2 l_5 & l_2 l_6 \\ l_3 l_1 & l_3 l_2 & l_3 l_3 & l_3 l_4 & l_3 l_5 & l_3 l_6 \\ l_4 l_1 & l_4 l_2 & l_4 l_3 & l_4 l_4 & l_4 l_5 & l_4 l_6 \\ l_5 l_1 & l_5 l_2 & l_5 l_3 & l_5 l_4 & l_5 l_5 & l_5 l_6 \\ l_6 l_1 & l_6 l_2 & l_6 l_3 & l_6 l_4 & l_6 l_5 & l_6 l_6 \end{bmatrix}$

Veronese mapping $V_{52} : P^5$ ! $P^{20}$, $V_{52}(P^5)$ $P^{20}$

Q is rank 1, det(Q) = 0, all 2 2 minors = 0, 210 (independent) quadratic equations

# Quadratic Constraint

$m \; ? \; d \; ) \quad l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$, quadratic in $l_i$, but linear in $l_i l_j$

Let $z = (l_1; l_2; l_3; l_4; l_5; l_6)$ and $Q = z^T z =$

$$\begin{bmatrix} l_1 l_1 & l_1 l_2 & l_1 l_3 & l_1 l_4 & l_1 l_5 & l_1 l_6 \\ l_2 l_1 & l_2 l_2 & l_2 l_3 & l_2 l_4 & l_2 l_5 & l_2 l_6 \\ l_3 l_1 & l_3 l_2 & l_3 l_3 & l_3 l_4 & l_3 l_5 & l_3 l_6 \\ l_4 l_1 & l_4 l_2 & l_4 l_3 & l_4 l_4 & l_4 l_5 & l_4 l_6 \\ l_5 l_1 & l_5 l_2 & l_5 l_3 & l_5 l_4 & l_5 l_5 & l_5 l_6 \\ l_6 l_1 & l_6 l_2 & l_6 l_3 & l_6 l_4 & l_6 l_5 & l_6 l_6 \end{bmatrix}$$

Veronese mapping $V_{52} : P^5 \; ! \; P^{20}$, $V_{52}(P^5) \quad P^{20}$

$Q$ is rank 1, $\det(Q) = 0$, all $2 \quad 2$ minors $= 0$, 210 (independent) quadratic equations

Formulate $y \; 2 \; R^{21}$ as the concatenation of upper triangular elements

$$y = [Q_{11}; :::; Q_{ij}; :::; Q_{66}]^T; \text{with } i \quad j$$

# Quadratic Constraint

m ? d ) $l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$, quadratic in $l_i$, but linear in $l_i l_j$

Let $z = (l_1; l_2; l_3; l_4; l_5; l_6)$ and $Q = z^T z =$

$$\begin{bmatrix} l_1 l_1 & l_1 l_2 & l_1 l_3 & l_1 l_4 & l_1 l_5 & l_1 l_6 \\ l_2 l_1 & l_2 l_2 & l_2 l_3 & l_2 l_4 & l_2 l_5 & l_2 l_6 \\ l_3 l_1 & l_3 l_2 & l_3 l_3 & l_3 l_4 & l_3 l_5 & l_3 l_6 \\ l_4 l_1 & l_4 l_2 & l_4 l_3 & l_4 l_4 & l_4 l_5 & l_4 l_6 \\ l_5 l_1 & l_5 l_2 & l_5 l_3 & l_5 l_4 & l_5 l_5 & l_5 l_6 \\ l_6 l_1 & l_6 l_2 & l_6 l_3 & l_6 l_4 & l_6 l_5 & l_6 l_6 \end{bmatrix}$$

Veronese mapping $V_{52} : P^5$ ! $P^{20}$, $V_{52}(P^5)$ $P^{20}$

Q is rank 1, det(Q) = 0, all 2 2 minors = 0, 210 (independent) quadratic equations

Formulate y 2 $R^{21}$ as the concatenation of upper triangular elements

$$y = [Q_{11}; \dots; Q_{ij}; \dots; Q_{66}]^T; \text{with } i \quad j$$

x = ( ; ; dim), with dim 2 f 1; 2; ...; 21g

# Quadratic Constraint

$Ay_i = b$, two constraints: $l_1 l_1 + l_2 l_2 + l_3 l_3 = 1$; $l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$

# Quadratic Constraint

$Ay_i = b$, two constraints: $l_1 l_1 + l_2 l_2 + l_3 l_3 = 1\,;\, l_1 l_4 + l_2 l_5 + l_3 l_6 = 0$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & \cdots & 0 & 0 & 0 \end{bmatrix}_{2 \times 21} \begin{bmatrix} l_1 l_1 \\ l_1 l_2 \\ l_1 l_3 \\ l_1 l_4 \\ l_1 l_5 \\ l_1 l_6 \\ l_2 l_2 \\ l_2 l_1 \\ \vdots \\ l_5 l_5 \\ l_5 l_6 \\ l_6 l_6 \end{bmatrix}_{21 \times 1} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

# Quadratic Constraint

$Ay_i = b$, two constraints: $l_1l_1 + l_2l_2 + l_3l_3 = 1\,;\, l_1l_4 + l_2l_5 + l_3l_6 = 0$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \quad & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & \quad & 0 & 0 & 0 \end{bmatrix}_{2\ 21} \begin{bmatrix} l_1l_1 \\ l_1l_2 \\ l_1l_3 \\ l_1l_4 \\ l_1l_5 \\ l_1l_6 \\ l_2l_2 \\ l_2l_1 \\ \vdots \\ l_5l_5 \\ l_5l_6 \\ l_6l_6 \end{bmatrix}_{21\ 1} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

For (x ) satis es A (x ) = b

# Quadratic Constraint

We don't want the 21D (x ) = y , but the 6D z .

# Quadratic Constraint

We don't want the 21D $(\mathbf{x})=\mathbf{y}$, but the 6D $\mathbf{z}$.

Problem: $\mathbf{Ay}=\mathbf{b}$ $(\ )$ $\mathbf{y}$ $2\,H1 \setminus H2$ in $\mathrm{R}^{21}$ (one hyperplane for every row in $\mathbf{A}$)

# Quadratic Constraint

We don't want the 21D $(\mathbf{x}) = \mathbf{y}$, but the 6D $\mathbf{z}$.

Problem: $\mathbf{A}\mathbf{y} = \mathbf{b}$ ( ) $\mathbf{y}$ 2 $H1 \setminus H2$ in $\mathbb{R}^{21}$ (one hyperplane for every row in $\mathbf{A}$)
$\dim(H1 \setminus H2) = 21 \quad 1 \quad 1 = 19$, $\dim(V_{52}(\mathbb{P}^5)) = 5$

# Quadratic Constraint

We don't want the 21D  ($\mathbf{x}$ ) = $\mathbf{y}$ , but the 6D $\mathbf{z}$ .

Problem: $\mathbf{A}\mathbf{y}$ = $\mathbf{b}$ ( ) $\mathbf{y}$ $2\; H1 \setminus H2$ in $\mathbb{R}^{21}$ (one hyperplane for every row in $\mathbf{A}$)
dim($H1 \setminus H2$) = 21  1  1 = 19, dim($V_{52}(\mathbb{P}^5)$) = 5
$9\mathbf{y}$ 62 $V_{52}(\mathbb{P}^5)$, let alone corresponding to point a on $M_2^4$ in $\mathbb{P}^5$!

# Quadratic Constraint

We don't want the 21D $(\mathbf{x}\ ) = \mathbf{y}$ , but the 6D $\mathbf{z}$ .

Problem: $\mathbf{Ay} = \mathbf{b}$ $(\ )$ $\mathbf{y}$ $2\ H1 \setminus H2$ in $\mathrm{R}^{21}$ (one hyperplane for every row in $\mathbf{A}$)

$\dim(H1 \setminus H2) = 21 \quad 1 \quad 1 = 19$, $\dim(V_{52}(\mathrm{P}^5)) = 5$

$9\mathbf{y}$ $62$ $V_{52}(\mathrm{P}^5)$, let alone corresponding to point a on $M_2^4$ in $\mathrm{P}^5$!

E.g.: (1 1 1 0 0 0 1 1 0 0 0 1 0 0 0 0 0 0 0 666 0)

# Quadratic Constraint

We don't want the 21D $(\mathbf{x}) = \mathbf{y}$, but the 6D $\mathbf{z}$.

Problem: $\mathbf{A}\mathbf{y} = \mathbf{b}$ ( ) $\mathbf{y} \in H1 \cap H2$ in $\mathbb{R}^{21}$ (one hyperplane for every row in $\mathbf{A}$)

$\dim(H1 \cap H2) = 21 \quad 1 \quad 1 = 19$, $\dim(V_{52}(\mathbb{P}^5)) = 5$

$\exists \mathbf{y} \notin V_{52}(\mathbb{P}^5)$, let alone corresponding to point a on $M_2^4$ in $\mathbb{P}^5$!

E.g.: (1 1 1 0 0 0 1 1 0 0 0 1 0 0 0 0 0 0 0 666 0)

$\mathbf{Q} = \mathbf{z}^T\mathbf{z}$ needs to be rank 1.

# Quadratic Constraint

We don't want the 21D $(\mathbf{x}) = \mathbf{y}$, but the 6D $\mathbf{z}$.

Problem: $\mathbf{Ay} = \mathbf{b}$ $(\ )$ $\mathbf{y}$ $2\ H1 \setminus H2$ in $\mathrm{R}^{21}$ (one hyperplane for every row in $\mathbf{A}$)
$\dim(H1 \setminus H2) = 21 \quad 1 \quad 1 = 19$, $\dim(V_{52}(\mathrm{P}^5)) = 5$
$9\mathbf{y}$ $2\!\!\!/\ V_{52}(\mathrm{P}^5)$, let alone corresponding to point a on $M_2^4$ in $\mathrm{P}^5$!
E.g.: (1 1 1 0 0 0 1 1 0 0 0 1 0 0 0 0 0 0 0 666 0)
$\mathbf{Q} = \mathbf{z}^T\mathbf{z}$ needs to be rank 1.

$$\mathbf{Q} = \begin{bmatrix} y_1 & y_2 & & y_6 \\ y_2 & y_7 & & y_{11} \\ \vdots & \vdots & \vdots & \vdots \\ y_6 & y_{11} & & y_{21} \end{bmatrix} = \mathbf{U}\ \mathbf{V}^T$$

# Quadratic Constraint

We don't want the 21D ($\mathbf{x}$) = $\mathbf{y}$, but the 6D $\mathbf{z}$.

Problem: $\mathbf{Ay} = \mathbf{b}$ ( ) $\mathbf{y}$ $2\ H1 \setminus H2$ in $R^{21}$ (one hyperplane for every row in $\mathbf{A}$)
$\dim(H1 \setminus H2) = 21 \quad 1 \quad 1 = 19$, $\dim(V_{52}(P^5)) = 5$
$9\mathbf{y}$ 2̸ $V_{52}(P^5)$, let alone corresponding to point a on $M_2^4$ in $P^5$!
E.g.: (1 1 1 0 0 0 1 1 0 0 0 1 0 0 0 0 0 0 0 666 0)
$\mathbf{Q} = \mathbf{z}^T\mathbf{z}$ needs to be rank 1.

$$\mathbf{Q} = \begin{bmatrix} y_1 & y_2 & & y_6 \\ y_2 & y_7 & & y_{11} \\ \vdots & \vdots & \vdots & \vdots \\ y_6 & y_{11} & & y_{21} \end{bmatrix} = \mathbf{U} \quad \mathbf{V}^T$$

$$\mathbf{z} = \sqrt{\quad_{(1;1)}}\,\mathbf{V}_{(:;1)}$$

# Quadratic Constraint

We don't want the 21D $(\mathbf{x}) = \mathbf{y}$, but the 6D $\mathbf{z}$.

Problem: $\mathbf{Ay} = \mathbf{b}$ ( ) $\mathbf{y} \in H1 \cap H2$ in $\mathbb{R}^{21}$ (one hyperplane for every row in $\mathbf{A}$)

$\dim(H1 \cap H2) = 21 \quad 1 \quad 1 = 19$, $\dim(V_{52}(\mathbb{P}^5)) = 5$

$\exists \mathbf{y} \notin V_{52}(\mathbb{P}^5)$, let alone corresponding to point a on $M_2^4$ in $\mathbb{P}^5$!

E.g.: (1 1 1 0 0 0 1 1 0 0 0 1 0 0 0 0 0 0 0 666 0)

$\mathbf{Q} = \mathbf{z}^T\mathbf{z}$ needs to be rank 1.

$$\mathbf{Q} = \begin{bmatrix} y_1 & y_2 & \cdots & y_6 \\ y_2 & y_7 & \cdots & y_{11} \\ \vdots & \vdots & \ddots & \vdots \\ y_6 & y_{11} & \cdots & y_{21} \end{bmatrix} = \mathbf{U}\ \ \mathbf{V}^T$$

$$\mathbf{z} = \sqrt{\ \ _{(1,1)}}\ \mathbf{V}_{(:,1)}$$

Sign ambiguity can be solved from context.

# No free lunch

$$O(n^3)$$

# No free lunch

$$O(n^3)$$

$$n = 81 \Rightarrow n \cdot 21 = 1701$$

University of Antwerp
Faculty of Applied Engineering

# No free lunch

$$O(n^3)$$

$n = 81$ ) $n$ 21 = 1701

6 2D GPs, 6 predictions per line

)

1 3D GP, 21 predictions per line plus SVD

# The problem with vanilla GPs

The posterior is a GP!!!

**Problem locally**: A prediction at $\mathbf{x}$ is a Gaussian distribution, ranging from $-\infty$ to $+\infty$. What about velocities, weights, heights, concentrations in %, ... ?

**Problem globally**: Kernel determines shape of the functions. Samples from posterior don't automatically obey monotonicity, convexity, boundary conditions, differential equations (heat, forces, ...), ...

**Problem multi-output**: Relationships between outputs are not built-in. What about zero curl or divergence in a vector field? What about unit norm vectors?

What about your data? **Does it matter**?

# Further reading

Swiler, L. P., Gulian, M., Frankel, A. L., Safta, C., & Jakeman, J. D. (2020). **A survey of constrained Gaussian process regression: Approaches and implementation challenges.** Journal of Machine Learning for Modeling and Computing, 1(2).

Salzmann, M., & Urtasun, R. (2010). **Implicitly constrained Gaussian process regression for monocular non-rigid pose estimation.** Advances in neural information processing systems, 23.

De Boi, I., Sels, S., De Moor, O., Vanlanduit, S., & Penne, R. (2022). **Input and output manifold constrained Gaussian process regression for galvanometric setup calibration.** IEEE Transactions on Instrumentation and Measurement, 71, 1-8.

InViLab

ivan.deboi@uantwerpen.be