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Linearly and nonlinearly constrained Gaussian processes

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Joint work with
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WASP ML Cluster,
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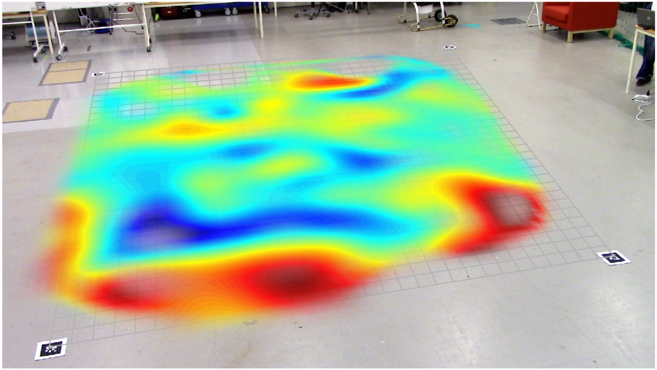
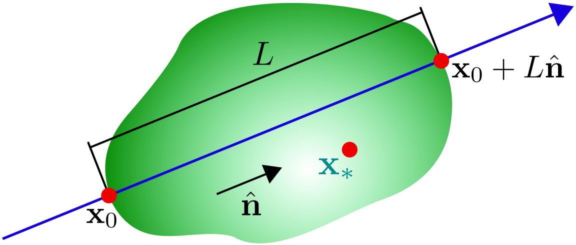
Motivation - Application 1:
Magnetic mapping - Indoor localization



Goal: Model magnetic field with a Gaussian process and infer measurements of this field

Question: Can we use any Maxwell's equations to constrain this model?

Motivation - Application 2: Strain field reconstruction



$$y = \mathcal{L}_{\mathbf{x}}\boldsymbol{\epsilon}(\mathbf{x}) + \varepsilon = \frac{1}{L}\int_0^L \hat{\mathbf{n}}^{\mathsf{T}}\boldsymbol{\epsilon}(\mathbf{x}^0 + s\hat{\mathbf{n}})\hat{\mathbf{n}}\, ds + \varepsilon$$

Goal: Model $\boldsymbol{\epsilon}(\mathbf{x})$ with a Gaussian process and infer the value of $\boldsymbol{\epsilon}(\mathbf{x}_*)$

Question: Can we use any physical knowledge to constrain this model?

Outline

Aim: Introduce constrained Gaussian process regression and demonstrate it on a few examples.

1. **GP basics**
2. Linear constraints
3. Strain field reconstruction
4. Nonlinear constraints

GP basics

Distribution over functions

$$\begin{bmatrix} f(\mathbf{x}_1) \\ \vdots \\ f(\mathbf{x}_N) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mu(\mathbf{x}_1) \\ \vdots \\ \mu(\mathbf{x}_N) \end{bmatrix}, \underbrace{\begin{bmatrix} k(\mathbf{x}_1, \mathbf{x}_1) & \cdots & k(\mathbf{x}_1, \mathbf{x}_N) \\ \vdots & & \vdots \\ k(\mathbf{x}_N, \mathbf{x}_1) & \cdots & k(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}}_{K} \right)$$

Gram matrix

Uniquely specified by mean and covariance function

$$\mu(\mathbf{x}_i) = \mathbb{E}\left[f(\mathbf{x}_i)\right]$$

$$k(\mathbf{x}_i, \mathbf{x}_j) = \mathrm{Cov}\left[f(\mathbf{x}_i),\ f(\mathbf{x}_j)\right]$$

Formally

$$f(\mathbf{x}) \sim \mathcal{GP}\left(\mu(\mathbf{x}),\ k(\mathbf{x}, \mathbf{x}')\right)$$

GP basics – prediction

Let

$$y_i = f(\mathbf{x}_i) + \varepsilon, \qquad \varepsilon \sim \mathcal{N}\left(0,\ \sigma^2\right)$$

$$\mathbf{y} = [y_1, y_2 \ldots, y_N]^\mathsf{T}$$

Then

$$\begin{bmatrix} \mathbf{y} \\ f(\mathbf{x}_*) \end{bmatrix} \sim \mathcal{N}\left(\begin{bmatrix} \mathbf{0} \\ 0 \end{bmatrix}, \begin{bmatrix} K + \sigma^2 I & \mathbf{k} \\ \mathbf{k}^\mathsf{T} & k(\mathbf{x}_*, \mathbf{x}_*) \end{bmatrix} \right)$$

$$K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$$

$$\mathbf{k}_i = k(\mathbf{x}_i, \mathbf{x}_*)$$

and

$$\mathbb{E}\left[f(\mathbf{x}_*)|\mathbf{y}\right] = \mathbf{k}^\mathsf{T}(K + \sigma^2 I)^{-1}\mathbf{y}$$

$$\mathbb{V}\left[f(\mathbf{x}_*)|\mathbf{y}\right] = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{k}^\mathsf{T}(K + \sigma^2 I)^{-1}\mathbf{k}$$

GP basics – linear operator measurements

Linear operator measurements

$$y = \mathcal{L}_{\mathbf{x}} f(\mathbf{x}) + \varepsilon$$

Then

$$\mathbb{E}\left[f(\mathbf{x}_*)|\mathbf{y}\right] = \mathbf{q}^{\mathsf{T}}(Q + \sigma^2 I)^{-1}\mathbf{y}$$
$$\mathbb{V}\left[f(\mathbf{x}_*)|\mathbf{y}\right] = k(\mathbf{x}_*, \mathbf{x}_*) - \mathbf{q}^{\mathsf{T}}(Q + \sigma^2 I)^{-1}\mathbf{q}$$

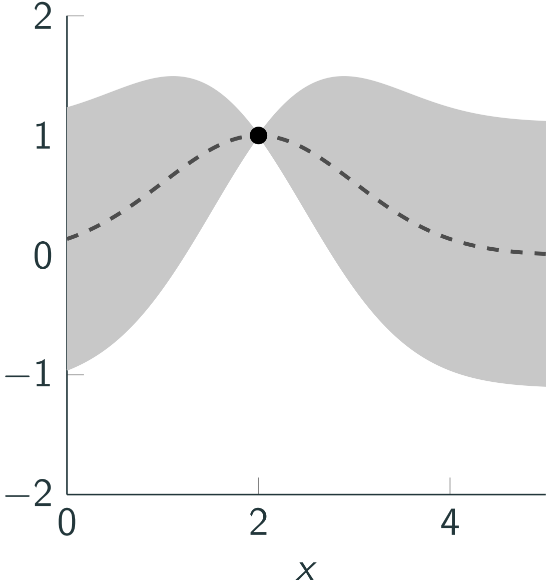
where

$$Q_{ij} = \mathcal{L}_{\mathbf{x}_i}\mathcal{L}_{\mathbf{x}_j} k(\mathbf{x}_i, \mathbf{x}_j)$$
$$\mathbf{q}_i = \mathcal{L}_{\mathbf{x}_i} k(\mathbf{x}_i, \mathbf{x}_*)$$

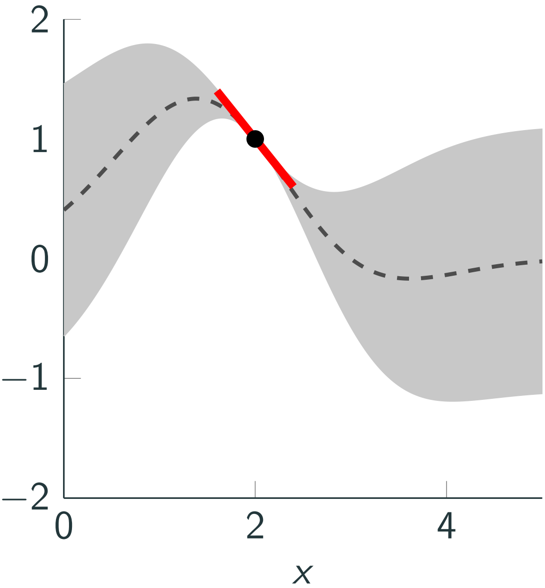
Example:

$$y_i = \int_{a_i}^{b_i} f(x)dx \quad \Rightarrow \begin{cases} Q_{ij} = \int_{a_i}^{b_i}\int_{a_j}^{b_j} k(x, x')\, dx'\, dx \\ \mathbf{q}_i = \int_{a_i}^{b_i} k(x, x_*)\, dx \end{cases}$$

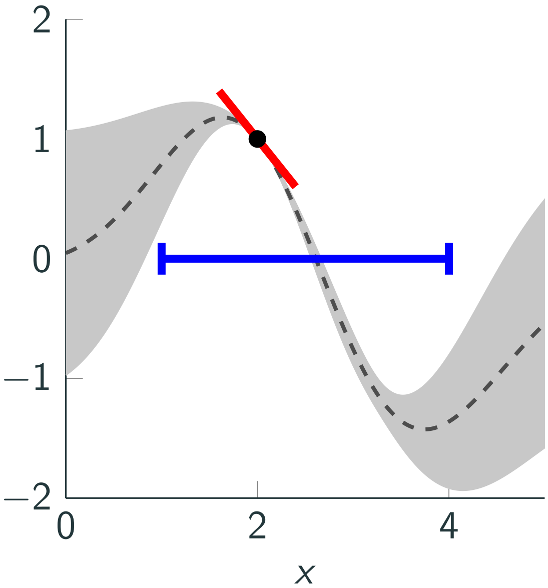
GP basics – linear operator measurements



GP basics – linear operator measurements



GP basics – linear operator measurements



Outline

1. GP basics
2. **Linear constraints**
3. Strain field reconstruction
4. Nonlinear constraints

Multivariate GP – constraint incorporation

Toy Example

Consider a Gaussian process

$$\mathbf{f}(\mathbf{x}) \sim \mathcal{GP}\left(\boldsymbol{\mu}(\mathbf{x}),\ \mathbf{K}(\mathbf{x}, \mathbf{x}')\right)$$

with two-dimensional input and two-dimensional output

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix}, \qquad \mathbf{x} = \begin{bmatrix} x \\ y \end{bmatrix}$$

Assume that we know from the physics that the all samples from the GP prior should obey the constraint

$$\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} = 0 \quad \Leftrightarrow \quad \underbrace{\begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix}}_{\mathscr{F}_{\mathbf{x}}} \mathbf{f}(\mathbf{x}) = 0$$

How can we model the covariance function $\mathbf{K}(\mathbf{x}, \mathbf{x}')$ such that this constraint is guaranteed to be obeyed?

Multivariate GP – constraint incorporation

Assume linear constraints

$$\mathscr{F}_{\mathbf{x}}\mathbf{f}(\mathbf{x}) = \mathbf{0}$$

Let $\mathbf{f}(\mathbf{x}) = \mathscr{G}_{\mathbf{x}}\mathbf{g}(\mathbf{x})$, where $\mathbf{g}(\mathbf{x}) \sim \mathcal{GP}\left(\boldsymbol{\mu}_{\mathbf{g}}(\mathbf{x}),\ \mathbf{K}_{\mathbf{g}}(\mathbf{x}, \mathbf{x}')\right)$

$$\mathbf{f}(\mathbf{x}) = \mathscr{G}_{\mathbf{x}}\mathbf{g}(\mathbf{x}) \sim \mathcal{GP}\left(\mathscr{G}_{\mathbf{x}}\ \boldsymbol{\mu}_{\mathbf{g}}(\mathbf{x}),\ \mathscr{G}_{\mathbf{x}}\mathbf{K}_{\mathbf{g}}(\mathbf{x}, \mathbf{x}')\mathscr{G}_{\mathbf{x}'}^{\mathsf{T}}\right)$$

Then

$$\mathscr{F}_{\mathbf{x}}\mathscr{G}_{\mathbf{x}}\mathbf{g}(\mathbf{x}) = \mathbf{0}$$

Arbitrary $\mathbf{g}(\mathbf{x})$

$$\Rightarrow \mathscr{F}_{\mathbf{x}}\mathscr{G}_{\mathbf{x}} = \mathbf{0}$$

Find $\mathscr{G}_{\mathbf{x}}$

Carl Jidling, Niklas Wahlstöm, Adrian Wills, Thomas B. Schön. **Linearly constrained Gaussian processes**. *Advances in Neural Information Processing Systems (NIPS)*,Long Beach, CA, USA, December, 2017.

Multivariate GP – constraint incorporation

Toy Example (cont.)

We consider the function

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_1(\mathbf{x}) \\ f_2(\mathbf{x}) \end{bmatrix}, \qquad \mathbf{x} = \begin{bmatrix} x \\ y \end{bmatrix}$$

and the constraint

$$\frac{\partial f_1}{\partial x} + \frac{\partial f_2}{\partial y} = 0 \quad \Leftrightarrow \quad \underbrace{\begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix}}_{\mathscr{F}_{\mathbf{x}}} \mathbf{f}(\mathbf{x}) = 0$$

Need $\mathscr{G}_{\mathbf{x}}$ such that $\mathscr{F}_{\mathbf{x}}\mathscr{G}_{\mathbf{x}} = \mathbf{0}$. One option is

$$\mathscr{G}_{\mathbf{x}} = \begin{bmatrix} -\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} \end{bmatrix}$$

since

$$\mathscr{F}_{\mathbf{x}}\mathscr{G}_{\mathbf{x}} = \begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix} \begin{bmatrix} -\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} \end{bmatrix} = -\frac{\partial^2}{\partial x \partial y} + \frac{\partial^2}{\partial y \partial x} = 0.$$

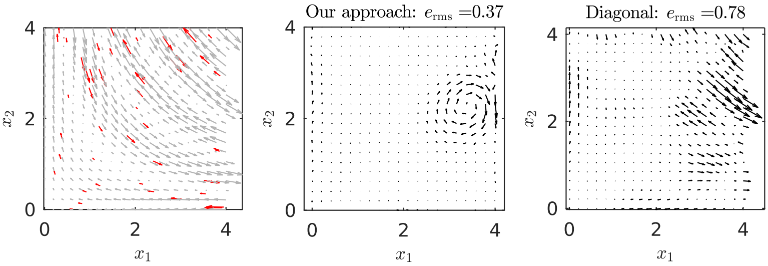
Simulation experiment - toy example

Choose $k_{\mathbf{g}}(\mathbf{x}, \mathbf{x}') = \sigma_f^2 e^{-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2l^2}}$. Then we get

$$\mathbf{K}(\mathbf{x}, \mathbf{x}') = \mathcal{G}_{\mathbf{x}} \mathcal{G}_{\mathbf{x}'}^{\mathsf{T}} k_{\mathbf{g}}(\mathbf{x}, \mathbf{x}') = \begin{bmatrix} -\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} \end{bmatrix} \begin{bmatrix} -\frac{\partial}{\partial y} & \frac{\partial}{\partial x} \end{bmatrix} k_{\mathbf{g}}(\mathbf{x}, \mathbf{x}')$$

$$= \sigma_f^2 e^{-\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{2l^2}} \left(\left(\frac{\mathbf{x}-\mathbf{x}'}{l} \right) \left(\frac{\mathbf{x}-\mathbf{x}'}{l} \right)^{\mathsf{T}} - \left(1 - \frac{\|\mathbf{x}-\mathbf{x}'\|^2}{l^2} \right) I_2 \right)$$

Below we have simulated a field which we know fulfills the constraint



Outline

1. **GP basics**
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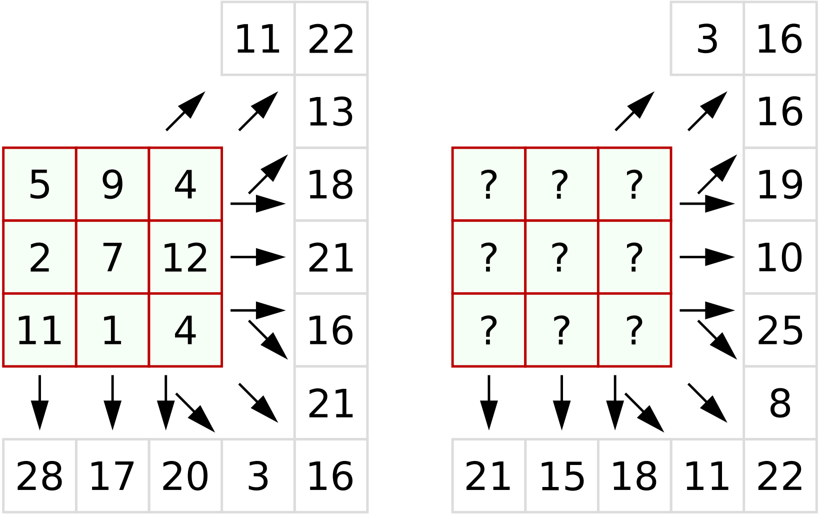
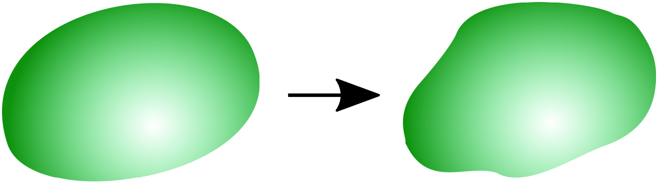
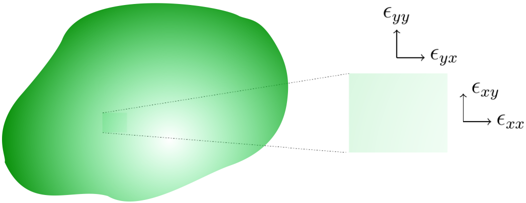
Tomography intuition



Strain field reconstruction

Deformed object

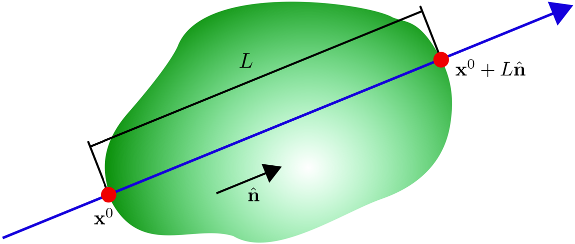




Reconstruct the *strain tensor*

$$\boldsymbol{\epsilon}(\mathbf{x}) = \begin{bmatrix} \epsilon_{xx}(\mathbf{x}) & \epsilon_{xy}(\mathbf{x}) \\ \epsilon_{xy}(\mathbf{x}) & \epsilon_{yy}(\mathbf{x}) \end{bmatrix}$$

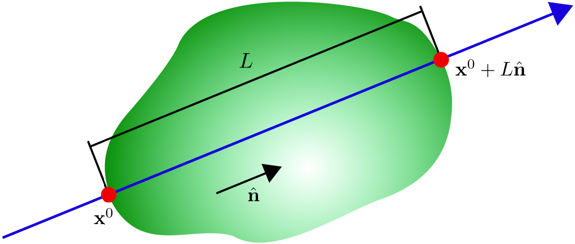
Strain field reconstruction



$$y = \frac{1}{L}\int_0^L \hat{\mathbf{n}}^\mathsf{T}\boldsymbol{\epsilon}(\mathbf{x}^0 + s\hat{\mathbf{n}})\hat{\mathbf{n}}\, ds + \varepsilon$$

$$\hat{\mathbf{n}} = \begin{bmatrix} n_x \\ n_y \end{bmatrix}, \qquad \varepsilon \sim \mathcal{N}(0, \sigma^2)$$

Strain field reconstruction



Vectorised form

$$y = \frac{1}{L}\int_0^L \vec{\mathbf{n}}^\mathsf{T}\mathbf{f}(\mathbf{x}^0 + s\hat{\mathbf{n}})\,ds + \varepsilon = \mathcal{L}_\mathbf{x}\mathbf{f}(\mathbf{x}^0) + \varepsilon$$

$$\mathbf{f}(\mathbf{x}) = \begin{bmatrix} f_{xx}(\mathbf{x}) \\ f_{xy}(\mathbf{x}) \\ f_{yy}(\mathbf{x}) \end{bmatrix} = \begin{bmatrix} \epsilon_{xx}(\mathbf{x}) \\ \epsilon_{xy}(\mathbf{x}) \\ \epsilon_{yy}(\mathbf{x}) \end{bmatrix}, \qquad \vec{\mathbf{n}} = \begin{bmatrix} n_x^2 \\ 2n_x n_y \\ n_y^2 \end{bmatrix}$$

Strain field reconstruction – constraint incorporation

A physical strain field must satisfy the *equilibrium constraints*

$$0 = \frac{\partial f_{xx}(\mathbf{x})}{\partial x} + (1-\nu)\frac{\partial f_{xy}(\mathbf{x})}{\partial y} + \nu\frac{\partial f_{yy}(\mathbf{x})}{\partial x}$$
$$0 = \nu\frac{\partial f_{xx}(\mathbf{x})}{\partial y} + (1-\nu)\frac{\partial f_{xy}(\mathbf{x})}{\partial x} + \frac{\partial f_{yy}(\mathbf{x})}{\partial y}$$

These can be written as

$$\mathbf{0} = \underbrace{\begin{bmatrix} \frac{\partial}{\partial x} & (1-\nu)\frac{\partial}{\partial y} & \nu\frac{\partial}{\partial x} \\ \nu\frac{\partial}{\partial y} & (1-\nu)\frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix}}_{\mathscr{F}_{\mathbf{x}}} \mathbf{f}(\mathbf{x})$$

Strain field reconstruction – constraint incorporation

We get

$$\mathcal{G}_{\mathbf{x}} = \begin{bmatrix} \frac{\partial^2}{\partial y^2} - \nu \frac{\partial^2}{\partial x^2} \\ -(1+\nu)\frac{\partial^2}{\partial x \partial y} \\ \frac{\partial^2}{\partial x^2} - \nu \frac{\partial^2}{\partial y^2} \end{bmatrix}$$

Hence

$$\mathbf{f}(\mathbf{x}) = \mathcal{G}_{\mathbf{x}} g(\mathbf{x})$$

Now let

$$g(\mathbf{x}) \sim \mathcal{GP}\left(0,\ k_g(\mathbf{x}, \mathbf{x}')\right)$$

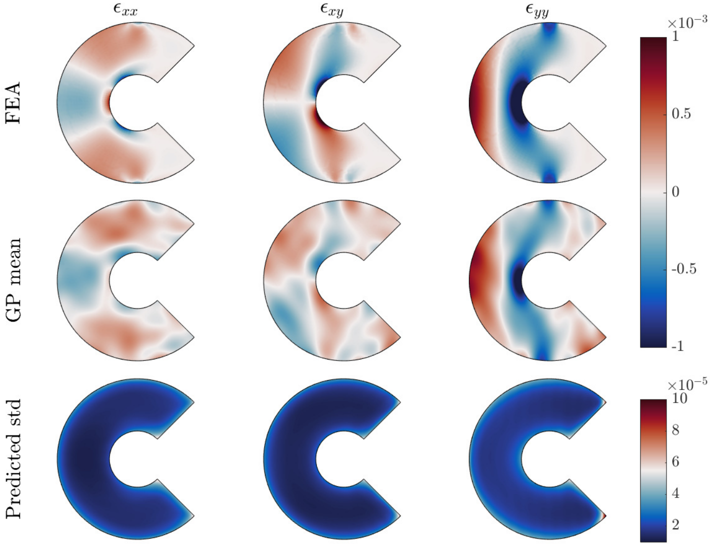
Then

$$\mathbf{f}(\mathbf{x}) \sim \mathcal{GP}\left(\mathbf{0},\ \mathcal{G}_{\mathbf{x}} \mathcal{G}_{\mathbf{x}'}^{\top} k_g(\mathbf{x}, \mathbf{x}')\right)$$

Note

$$y = \mathcal{L}_{\mathbf{x}}[\mathcal{G}_{\mathbf{x}} g(\mathbf{x})] + \varepsilon$$

Strain field reconstruction – experimental results



Carl Jidling, Johannes Hendriks, Niklas Wahlström, Alexander Gregg, Thomas B. Schön, Chris Wensrich, Adrian Wills. **Probabilistic modelling and reconstruction of strain**, *Nuclear instruments and methods in physics research section B*, 436:141-155, 2018.

Outline

1. GP basics
2. Linear constraints
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Nonlinearly constrained Gaussian processes- idea

Question: What can we do if we have nonlinear constraints?

We focus on sum-constrained Gaussian processes

$$\mathcal{F}[\mathbf{f}(\mathbf{x})] = \sum_i a_i h_i(f_i(\mathbf{x})) = C,$$

where $h_i(\cdot)$ is a non-linear function.

Idea: Reduce nonlinear constraints to linear

$$\mathcal{F}[\mathbf{f}'(\mathbf{x})] = \sum a_i f_i'(\mathbf{x}) = C, \qquad f_i' = h_i(f_i)$$

1. Train constrained GP f' on transformed data $y_i' = h_i(y_i)$
2. Subsequently backtransform constrain GP $f_i = h_i^{-1}(f_i')$

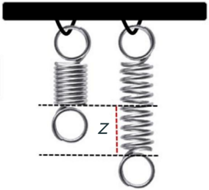
Note: Note, since h_i is nonlinear we do not enjoy Gaussian property anymore. We use Laplace approximation to deal with this.

Nonlinearly constrained Gaussian processes- toy example

Toy Example (harmonic oscillator)

Motion modelled by multitask Gaussian process

$$\mathbf{f}(t) = \begin{bmatrix} f_z(t) \\ f_v(t) \end{bmatrix} \qquad \begin{matrix} z : \text{displacement} \\ v : \text{velocity} \end{matrix}$$



Constraint: energy conservation (friction neglected)

$$E = E_{\mathrm{pot}}(t) + E_{\mathrm{kin}}(t) = \frac{k}{2} f_z(t)^2 + \frac{m}{2} f_v(t)^2,$$

Sum constraint parameters

$$\mathcal{F}[\mathbf{f}(\mathbf{x})] = \sum_i a_i h_i(f_i(\mathbf{x})) = C,$$

$$a_1 = k/2, \quad h_1(f_z) = f_z^2$$
$$a_2 = m/2, \quad h_2(f_v) = f_v^2, \quad C = E.$$

Nonlinearly constrained Gaussian processes- auxiliary variables

Problem h_i has to be (piecewise) invertible

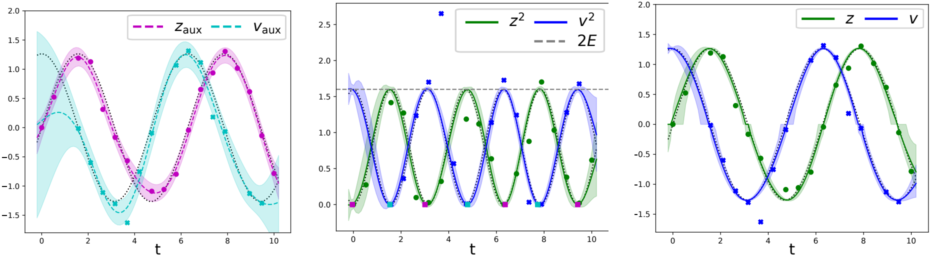
Solution Add auxiliary variables to make invertible

Ex Toy Example (harmonic oscillator) Auxiliary variables: z and v

1. Train constrained GP $f' = [f'_{z^2}, f'_{v^2}, f'_z, f'_v]$ on transformed data $\mathbf{y}' = [z^2, v^2, z, v]^T$
2. Subsequently backtransform constrained GP

$$f_z = \text{sign}(f'_z)\sqrt{f'_{z^2}}$$
$$f_v = \text{sign}(f'_v)\sqrt{f'_{v^2}}$$

Nonlinearly constrained Gaussian processes - toy example



Left: Results for unconstrained GP

Middle: Results for transformed output learned by the constrained GP

Right: The back transformed output. The results for the unconstrained GP are used to recover the signs.

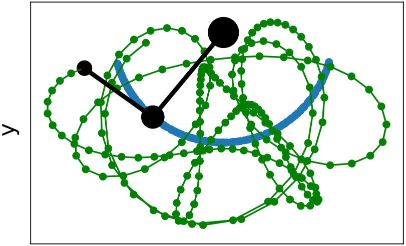
Nonlinearly constrained Gaussian processes - Double pendulum (real data)

Real data example (double pendulum)

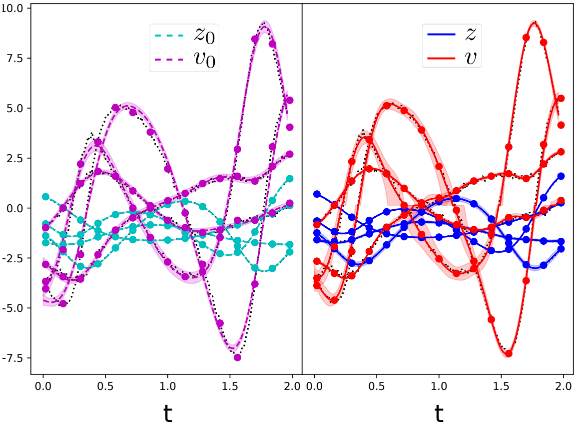
We model both positions z_x, z_y and velocities v_x, v_y of the two masses, (i.e. 8 outputs), while at the same time respecting the law of energy conservation

$$E = m_b g z_{by} + m_g g z_{gy} + \frac{m_b}{2}\left(v_{bx}^2 + v_{by}^2\right) + \frac{m_g}{2}\left(v_{gx}^2 + v_{gy}^2\right),$$

Indices b and g refer to blue and green pendulum, respectively.



Nonlinearly constrained Gaussian processes - Double pendulum (real data) - Results



Left: Results for unconstrained GP **Right:** Results for constrained GP

Philipp Pilar, Carl Jidling, Thomas B. Schön, Niklas Wahlström. **Incorporating sum constraints into multitask Gaussian processes**, *arXiv preprint arXiv:1504.00702*, 2022.

Conclusions and references

- Linear constraints can be incorporated in Gaussian processes
- Promising results on simulated and real data experiments
- The idea can also be extended to a nonlinear constraints

References

Carl Jidling, Niklas Wahlstöm, Adrian Wills, Thomas B. Schön. **Linearly constrained Gaussian processes**. *Advances in Neural Information Processing Systems (NIPS)*,Long Beach, CA, USA, December, 2017.

Arno Solin, Manon Kok, Niklas Wahlström, Thomas B. Schön, and Simo Särkkä. **Modeling and interpolation of the ambient magnetic field by Gaussian processes**. *IEEE Transactions on Robotics*, 34(4):1112 – 1127, 2018

Carl Jidling, Johannes Hendriks, Niklas Wahlström, Alexander Gregg, Thomas B. Schön, Chris Wensrich, Adrian Wills. **Probabilistic modelling and reconstruction of strain**, *Nuclear instruments and methods in physics research section B*, 436:141-155, 2018.

Philipp Pilar, Carl Jidling, Thomas B. Schön, Niklas Wahlström. **Incorporating sum constraints into multitask Gaussian processes**, *Transactions on Machine Learning Research*, 2022.

Backup slides

Algorithm idea – toy example

Step 1: Assume that $\mathcal{G}_{\mathbf{x}}$ contains the same operators as $\mathcal{F}_{\mathbf{x}}$

$$\mathcal{G}_{\mathbf{x}} = \begin{bmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{21} & \gamma_{22} \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{bmatrix}$$

Step 2: Expand

$$\mathcal{F}_{\mathbf{x}} \mathcal{G}_{\mathbf{x}} = \begin{bmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix} \begin{bmatrix} \gamma_{11} & \gamma_{12} \\ \gamma_{21} & \gamma_{22} \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{bmatrix}$$

$$= \gamma_{11} \frac{\partial^2}{\partial x^2} + (\gamma_{12} + \gamma_{21}) \frac{\partial^2}{\partial x \partial y} + \gamma_{22} \frac{\partial^2}{\partial y^2}$$

Algorithm idea – toy example

Step 3: We need

$$\begin{cases} \gamma_{11} &= 0 \\ \gamma_{12} &= -\gamma_{21} \\ \gamma_{22} &= 0 \end{cases}$$

Step 4: Choosing $\gamma_{21} = 1$, we get

$$\mathcal{G}_{\mathbf{x}} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \end{bmatrix} = \begin{bmatrix} -\frac{\partial}{\partial y} \\ \frac{\partial}{\partial x} \end{bmatrix}$$

No solution? Retry with higher order operators!

Even more formal treatment based on polynomial rings and Gröbner basis theory is published in

Markus Lange-Hegermann. **Algorithmic Linearly Constrained Gaussian Processes**, *Advances in Neural Information Processing Systems (NeurIPS)*, Montreal, 2018.