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# Probabilistic modelling – driven by data, guided by physics

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*"Machine learning gives computers the ability to* **learn without being explicitly programmed** *for the task at hand."*

# Machine Learning – the four cornerstones

Cornerstone 1 **(Data)** Typically we need lots of it.

Cornerstone 2 **(Mathematical model)** A mathematical model is a compact representation of the data that in precise mathematical form captures the key properties of the underlying situation.

Cornerstone 3 **(Learning algorithm)** Used to compute the unknown variables from the observed data using the model.

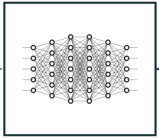
Cornerstone 4 **(Decision/Control)** Use the understanding of the current situation to steer it into a desired state.

# Ex – Automatic ECG classification

ECG data


*Input*, $\mathbf{x}$

Computer program



*Model*

$y \in \{$ `atrial fibrillation`, `sinus tachycardia`, `1st degree AV block`, $\ldots$

*Prediction*

We are now reaching human level (medical doctor) performance on certain specific tasks.

> **Key difference** to "classical engineering": The model is **not** derived based on our ability to mathematically explain what we see in an ECG.
>
> Instead, a generic model is **automatically learned** based on data.

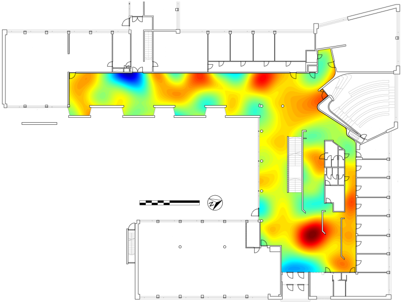
Ribeiro, A. H., Ribeiro, M. H., Paixao, G. M. M., Oliveira, D. M., Gomes, P. R., Canazart, J. A., Ferreira, M. P. S., Andersson, C. R., Macfarlane, P. W., Meira, W., TS and Ribeiro, A. L. P. **Automatic diagnosis of the short-duration 12-lead ECG using a deep neural network: the CODE study**, *arXiv:1904.01949*, 2019.

# Ex (Machine Learning) – Ambient magnetic field map

The Earth's magnetic field sets a background for the ambient magnetic field. Deviations make the field vary from point to point.

**Aim:** Build a map (i.e., a model) of the magnetic environment based on magnetometer measurements.

**Solution:** Customized Gaussian process that obeys Maxwell's equations.



www.youtube.com/watch?v=enlMiUqPVJo

Carl Jidling, Niklas Wahlström, Adrian Wills and TS. **Linearly constrained Gaussian processes**. *Advances in Neural Information Processing Systems (NeurIPS)*, Long Beach, CA, USA, December, 2017.

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

# Probabilistic modelling – representation of beliefs (uncertainty)

For a machine to behave intelligently I believe it needs the

**capability to represent and manipulate beliefs/uncertainty**

about the real world.

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As the machine perceives the world via its sensors it must then update its beliefs in light of the new information.

The mathematics of **probability theory** is well developed and

1. it allows us to not only **represent** uncertainty,
2. but it also prescribes how to **manipulate** it based on the information in new measurements.

# Probabilistic modelling – representation of beliefs (uncertainty)

A very important fact is that **inverse probability** (i.e. Bayes rule)

$$p(x \mid y) = \frac{p(y \mid x)p(x)}{p(y)}$$

allows us to infer unknown variables ($x$), adapt our models, make predictions and learn from data ($y$).

Ghahramani, Z. **Probabilistic machine learning and artificial intelligence**. *Nature* 521:452-459, 2015.

# Key lesson from contemporary Machine Learning

**Flexible models** often give the best performance.

How can we build and work with these flexible models?

1. Models that use a large (but fixed) number of parameters. (**parametric**, ex. deep learning)

   LeCun, Y., Bengio, Y., and Hinton, G. **Deep learning**, *Nature*, Vol 521, 436–444, 2015.

2. Models that use "more parameters" as we get access to more data. (**non-parametric**, ex. Gaussian process)

   Ghahramani, Z. **Probabilistic machine learning and artificial intelligence**. *Nature* 521:452-459, 2015.

# Blending prior knowledge and data

While we can do a lot with our data and flexible black-box models, we have already understood a lot about nature.

**What if we could combine the two?!**

Meaning that we start from small (rigid) models describing the phenomenon we are studying and augment them with flexible models driven by data.

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**Personal opinion:** I believe that there are (massive) gains to be made in the (simple) combination of flexible data-driven models and solid widely available knowledge that we already have.

**Aim of this talk:** Try to provide some concrete evidence for my opinion (and to mention the GP).

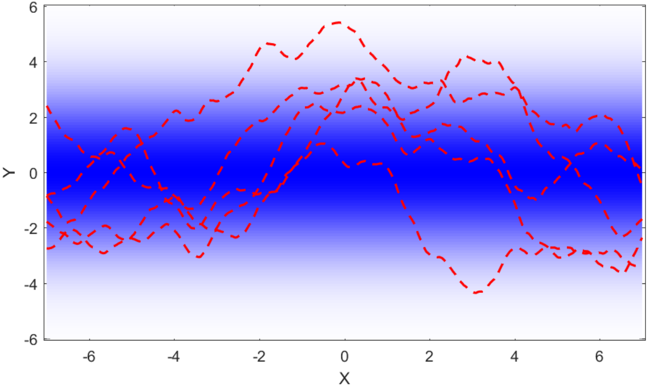
# The Gaussian process is a model for nonlinear functions

**Q:** Why is the Gaussian process used everywhere?

It is a **non-parametric** and **probabilistic** model for nonlinear functions.

- **Non-parametric** means that it does not rely on any particular parametric functional form to be postulated.
- **Probabilistic** means that it takes uncertainty into account in every aspect of the model.

# GP regression – illustration



# Starting somewhere – more concrete from hereon

**Fact:** Linear functional constraints and measurements are **useful** in describing nature and **simple** to work with.

Very specific examples:

1. The magnetic field $H$ is curl-free (recall example from before)

$$\nabla \times H = 0.$$

2. Measurements are expressed as line integrals of the target function
   - X-ray computed tomography (CT)
   - Strain field reconstruction from neutron diffraction experiments

| | | | |
|---|---|---|---|
| 2 | 16 | 13 | 3 |
| 11 | 5 | 8 | 10 |
| 7 | 9 | 12 | 6 |
| 14 | 4 | 1 | 15 |

| | | |
|---|---|---|
| 4 | 9 | 2 |
| 3 | 5 | 7 |
| 8 | 1 | 6 |

# Computed tomography (CT)

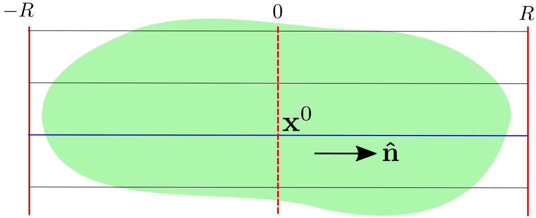
**Tomographic reconstruction:** Recover the internal structure

$$f(\mathbf{x}), \ \mathbf{x} = [x \ y]^\mathsf{T}$$

of an object from irradiation experiments.

Line integral measurements

$$y = \int_{-R}^{R} f(\mathbf{x}^0 + s\hat{\mathbf{n}})ds + \varepsilon, \qquad \varepsilon \sim \mathcal{N}(0, \sigma^2)$$




Limited data (sparse projections) important.

# Linear functional measurements in GPs (more general)

Model the target function $f(\mathbf{x})$ as a GP

$$f(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$$

Fact: a GP is closed under linear transformations:

$$\mathcal{L}f(\mathbf{x}) \sim \mathcal{GP}(0, \mathcal{L}\mathcal{L}'k(\mathbf{x}, \mathbf{x}'))$$

where for us (in the CT case)

$$\mathcal{L}f(\mathbf{x}) = \int_{-r}^{r} f(\mathbf{x}^0 + s\hat{\mathbf{n}})ds,$$

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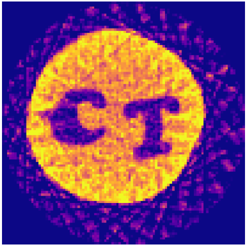
Our CT and strain field reconstruction examples have measurements:

$$y = \int_{-r}^{r} f(\mathbf{x}^0 + s\hat{\mathbf{n}})ds + \varepsilon, \qquad \varepsilon \sim \mathcal{N}(0, Q)$$

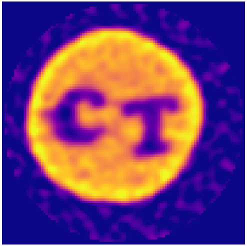
Carl Jidling, Niklas Wahlström, Adrian Wills and TS. **Linearly constrained Gaussian processes**. *Advances in Neural Information Processing Systems (NIPS)*, Long Beach, CA, USA, December, 2017.

# Ex. CT – carved cheese experiment

Ground truth



FBP



GP

**Question:** Why is the GP solution so blurry?

All details on this construction are available in

Zenith Purisha, Carl Jidling, Niklas Wahlström, Simo Särkkä, TS. **Probabilistic approach to limited-data computed tomography reconstruction**, *Inverse problems*, 2019.

# Extending the expressiveness to non-stationary behaviors

The covariance function $k(\mathbf{x}, \mathbf{x}')$, stipulates the basic behavior of the target function $f(\mathbf{x})$.

The selection of $k(\mathbf{x}, \mathbf{x}')$ is the most crucial part of GP modelling.

Extend the expressiveness of stationary covariance functions by transforming the inputs through a nonlinear mapping $u(\cdot)$ to form $k(u(\mathbf{x}), u(\mathbf{x}'))$, effectively opening up for non-stationary behaviors.

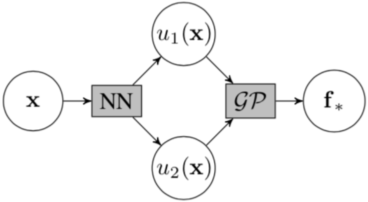
**Question:** Which mapping should we use?

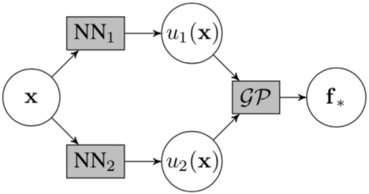
Let's try a deep neural network...


Andrew G.Wilson, Zhiting Hu, Ruslan R. Salakhutdinov, and Eric P. Xing. **Deep kernel learning**. In *Advances in Neural Information Processing Systems (NIPS)*, 2016.

Roberto Calandra, Jan Peters, Carl E. Rasmussen, and Marc P. Deisenroth. **Manifold Gaussian processes for regression**. In *Proceedings of the International Joint Conference on Neural Networks (IJCNN)*, 2016.

# One useful way of combining deep learning with GPs

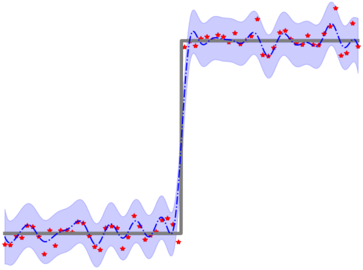


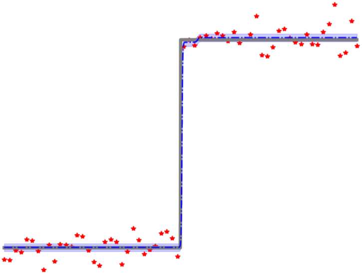

**Intuition:** The neural network does not have to learn the complete function $f(\mathbf{x})$, but only identify its discontinuities while for the remaining part the model can rely upon the regression capabilities of the GP.

# Ex. – illustrating the idea

$$k(x, x') = \sigma_f^2 e^{-\frac{1}{2l^2}(x-x')^2}$$

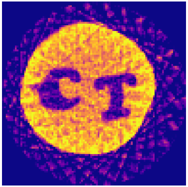


$$k(x, x') = \sigma_f^2 e^{-\frac{1}{2l^2}(u(x)-u(x'))^2}$$

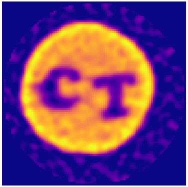


# Using the idea together with integral measurements

Ground truth



FBP



GP

GP + DL

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**GP + DL:** Deep learning to use the input mapping together with our taylored GP prior encoding our understanding of the underlying physics.

> **Vision:** Create flexible model building blocks containing the basic knowledge we have about the phenomenon we are studying.

# AI4theSciences – University-wide rapidly moving entity

At Uppsala University we will develop and make use of
**AI/ML for the sciences**.

A **time-limited five year effort** consisting of an
**antidisciplinary entity** from the entire university.

Key mechanism: **Internal AI sabbatical periods**

- Probably funded 50% by the entity and the rest by the department where the fellow remains employed/external grants.
- Duration: around 12 months.
- The fellows are expected to bring along one or several of their PhD students/post-docs to develop the ideas formed within the entity.
- Opens up for many of the positive aspects of doing a sabbatical.

# Conclusion

The **combined use** of data-driven flexible models and existing knowledge can be quite rewarding.

The best predictive performance is currently obtained from **highly flexible learning systems**.

We mainly used one flexible model class: Gaussian process (GP)

Hinted at how to embed basic knowledge from physics into the GP.

**Uncertainty** is a key concept!

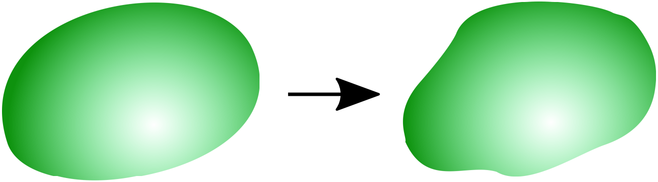
Remember to talk to people who work on **different problems** with **different tools**!! (Visit other fields!)

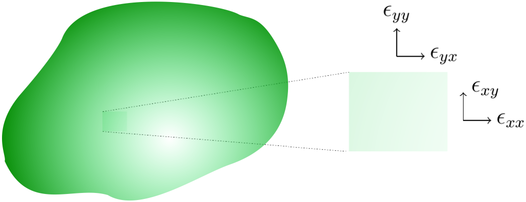
# Backup slides

# Strain field reconstruction – background

**Tomographic reconstruction:** Recover the internal structure of an object from irradiation experiments.

Deformed object



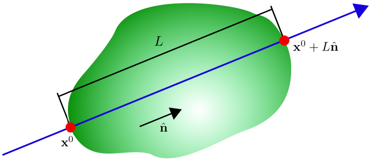



Reconstruct the **strain tensor**

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

# Strain field reconstruction – measurement model

Neutron beams are generated at a source, transmitted through the sample (along $\hat{\mathbf{n}}$) and recorded at a detector.




Measurement model (vectorised form):

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

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

# Strain field reconstruction – covariance model

Put a GP on the strain field $\mathbf{f}(\mathbf{x})$

$$\mathbf{f}(\mathbf{x}) \sim \mathcal{GP}(\mathbf{0}, \mathbf{K}(\mathbf{x}, \mathbf{x}'))$$

Since $\mathbf{f}(\mathbf{x})$ is multivariate, the covariance function is a **matrix**

$$\mathbf{K}(\mathbf{x}, \mathbf{x}') = \begin{bmatrix} k_{11}(\mathbf{x}, \mathbf{x}') & k_{12}(\mathbf{x}, \mathbf{x}') & k_{13}(\mathbf{x}, \mathbf{x}') \\ k_{21}(\mathbf{x}, \mathbf{x}') & k_{22}(\mathbf{x}, \mathbf{x}') & k_{23}(\mathbf{x}, \mathbf{x}') \\ k_{31}(\mathbf{x}, \mathbf{x}') & k_{32}(\mathbf{x}, \mathbf{x}') & k_{33}(\mathbf{x}, \mathbf{x}') \end{bmatrix}$$

How should we select $\mathbf{K}(\mathbf{x}, \mathbf{x}')$?

There are certain physical constraints that it needs to fulfill.

# Multivariate GP – constraint incorporation

Assume linear constraints

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

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

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

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 Wahlström, Adrian Wills and TS. **Linearly constrained Gaussian processes**. *Advances in Neural Information Processing Systems (NIPS)*, Long Beach, CA, USA, December, 2017.

# Multivariate GP – constraint incorporation

## Toy Example

Let

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

and consider the constraint

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

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

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

# Strain field reconstruction – constraint incorporation

A physical strain field must satisfy the **equilibrium constraints** (isotropic linear elastic solid materials under plain stress)

$$
\begin{aligned}
0 &= \frac{\partial f_{xx}(\mathbf{x})}{\partial x} + (1-\nu)\frac{\partial f_{xy}(\mathbf{x})}{\partial y} + \nu \frac{\partial f_{yy}(\mathbf{x})}{\partial x}, \\
0 &= \nu \frac{\partial f_{xx}(\mathbf{x})}{\partial y} + (1-\nu)\frac{\partial f_{xy}(\mathbf{x})}{\partial x} + \frac{\partial f_{yy}(\mathbf{x})}{\partial y}.
\end{aligned}
$$

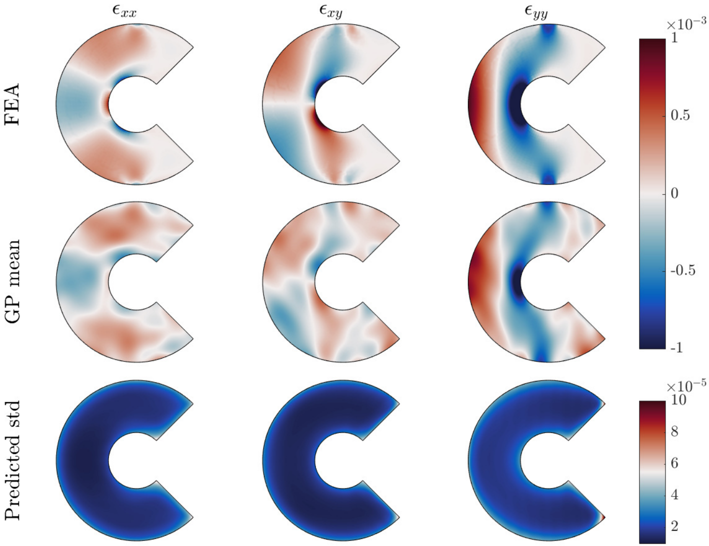
These can be written as

$$
\mathbf{0} = \underbrace{\begin{bmatrix} \frac{\partial}{\partial x} & (1-\nu)\frac{\partial}{\partial y} & \nu \frac{\partial}{\partial x} \\ \nu \frac{\partial}{\partial y} & (1-\nu)\frac{\partial}{\partial x} & \frac{\partial}{\partial y} \end{bmatrix}}_{\mathscr{F}_{\mathbf{x}}} \mathbf{f}(\mathbf{x}) = \begin{bmatrix} \boldsymbol{c}_1^{\mathsf{T}} \\ \boldsymbol{c}_2^{\mathsf{T}} \end{bmatrix} \mathbf{f}(\mathbf{x})
$$

We have constructed a Gaussian process that is **guaranteed to obey linear operator constraints** by shaping the covariance function

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

# Strain field reconstruction – experimental results




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