State Space Expectation Propagation

Efficient Inference Schemes for Temporal Gaussian Processes

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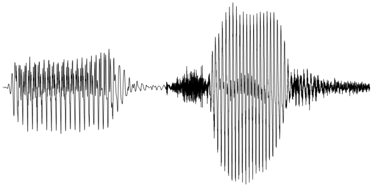
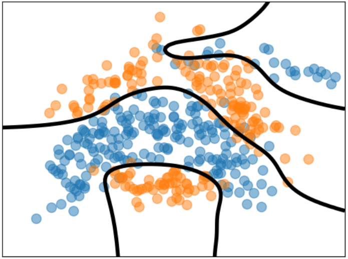
Aalto University

DTU

Motivation

- We're interested in long temporal and spatio-temporal data with interesting non-conjugate GP models (e.g. classification, log-Gaussian Cox processes).
- Idea: We should treat the temporal dimension in a fundamentally different manner to other dimensions.





Approximate Inference in Temporal GPs

There exists a dual kernel / SDE form for most popular Gaussian process (GP) models

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f(t) &\sim \mathcal{GP}\big(0,\, K_\theta(t,t')\big), & \mathbf{f}_k &= \mathbf{A}_{\theta,k}\mathbf{f}_{k-1} + \mathbf{q}_k, & \mathbf{q}_k &\sim \mathrm{N}(\mathbf{0}, \mathbf{Q}_k) \\
y_k &\sim p(y_k \mid f(t_k)) & y_k &= h(\mathbf{f}_k, \boldsymbol{\sigma}_k), & \boldsymbol{\sigma}_k &\sim \mathrm{N}(0, \boldsymbol{\Sigma}_k)
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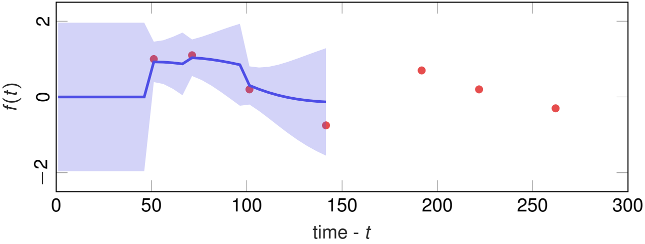
inference in $\mathcal{O}(n)$ via Kalman filtering and smoothing

Approximate Inference

Kalman filter update step:

$$p(\mathbf{f}_k|y_{1:k}) \propto \mathrm{N}(\mathbf{m}_k^{\text{predict}}, \mathbf{P}_k^{\text{predict}})\, p(y_k \mid f(t_k))$$



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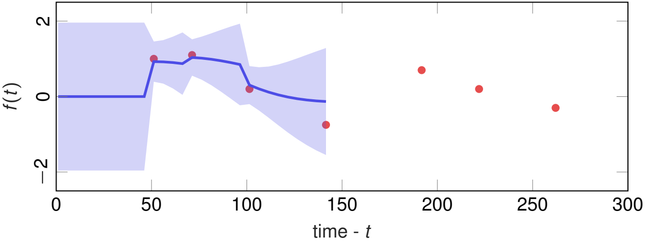

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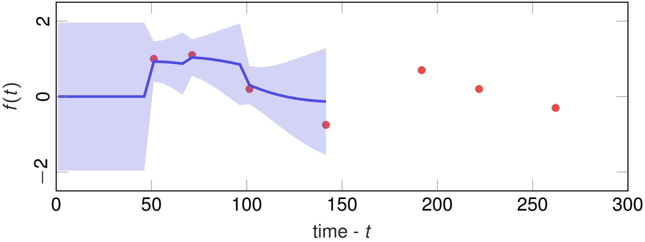

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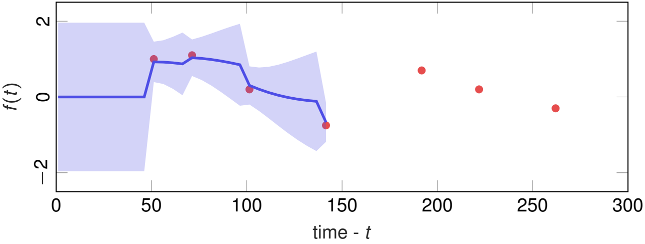

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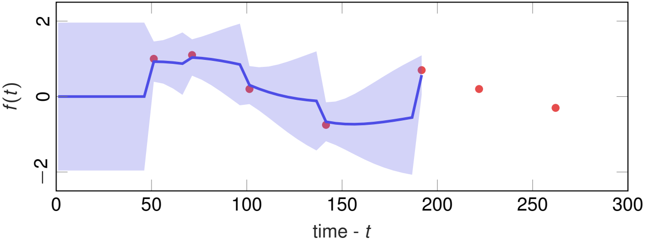

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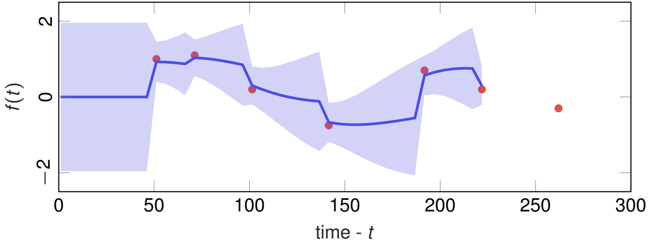

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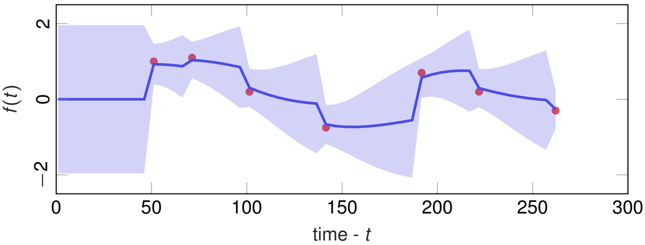

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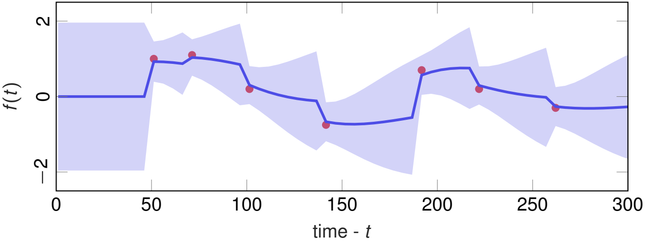

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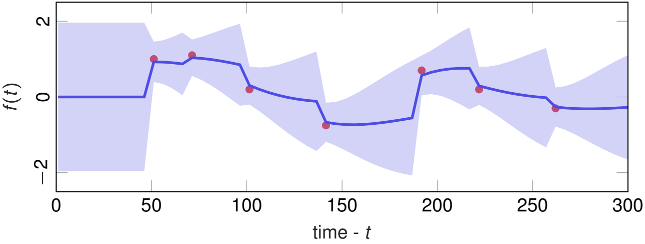

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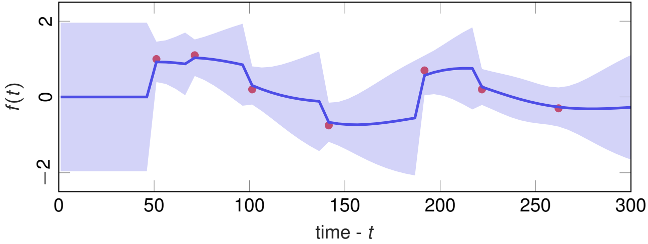

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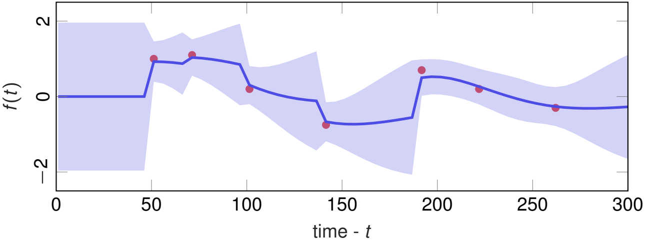

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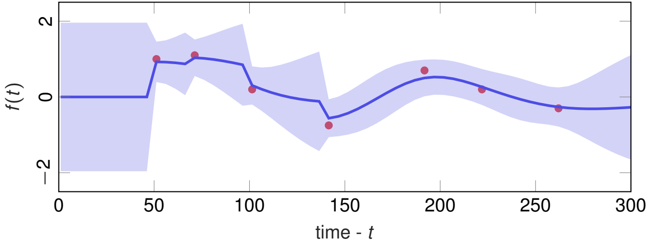

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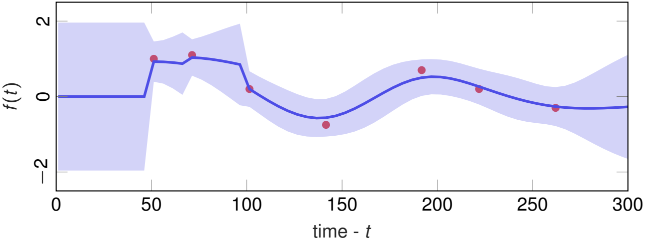

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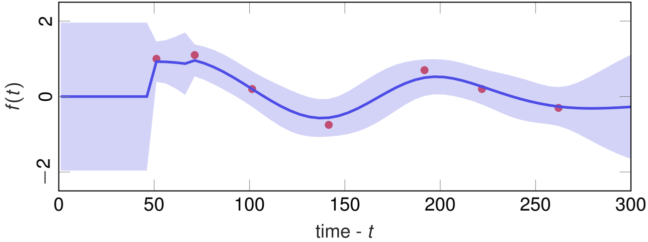

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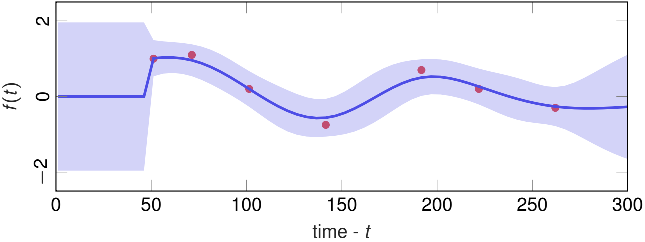

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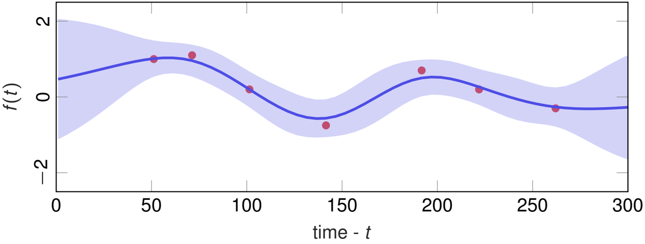

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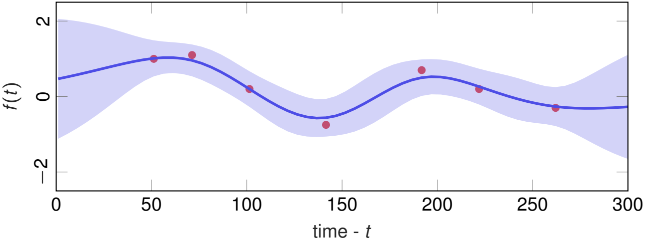
Given marginal posterior $\mathrm{N}(\mathbf{m}_k^{\text{post.}}, \mathbf{P}_k^{\text{post.}})$, we show how approximate inference amounts to a simple site parameter update rule during smoothing.



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This encompasses:

- Power Expectation Propagation
- Variational Inference (with natural gradients)
- Extended Kalman Smoothing
- Unscented / Gauss-Hermite Kalman Smoothing
- Posterior Linearisation

Parameter Update Rules

for $\nabla \mathcal{L}_k = \frac{\mathrm{d}\mathcal{L}_k}{\mathrm{d}\mathbf{m}_k}$

Power Expectation Propagation:

$$q_{\text{cavity}}(\mathbf{f}_k) = q_{\text{post.}}(\mathbf{f}_k) / q^{\alpha}_{\text{site}}(\mathbf{f}_k)$$

$$\mathcal{L}_k = \log \mathbb{E}_{q_{\text{cavity}}}\left[p^{\alpha}(\mathbf{y}_k \mid \mathbf{f}_k)\right]$$

$$\mathbf{P}^{\text{site}}_k = -\alpha\left(\mathbf{P}^{\text{cavity}}_k + \left(\nabla^2 \mathcal{L}_k\right)^{-1}\right)$$

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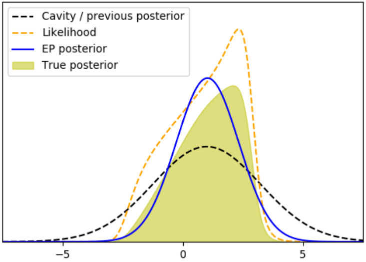

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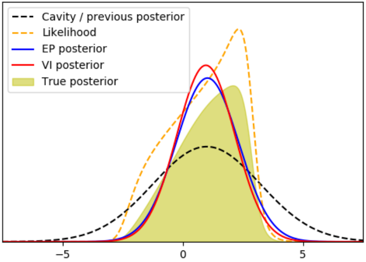

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Extended Kalman Smoother:

$$\mathbf{v}_k = \mathbf{y}_k - \mathbf{h}(\mathbf{m}^{\text{post.}}_k, \mathbf{0})$$

$$\mathbf{S}_k = \mathbf{H}_{\mathbf{f}}^{\top}\mathbf{P}^{\text{post.}}_k\mathbf{H}_{\mathbf{f}} + \mathbf{H}_{\boldsymbol{\sigma}}\Sigma_k\mathbf{H}_{\boldsymbol{\sigma}}^{\top}$$

$$\mathbf{P}^{\text{site}}_k = \left(\mathbf{H}_{\mathbf{f}}^{\top}\left(\mathbf{H}_{\boldsymbol{\sigma}}\Sigma_k\mathbf{H}_{\boldsymbol{\sigma}}^{\top}\right)^{-1}\mathbf{H}_{\mathbf{f}}\right)^{-1}$$

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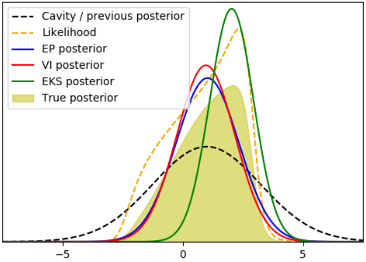

for $\mathbf{H}_{\mathbf{f}} = \frac{\mathrm{d}\mathbf{h}}{\mathrm{d}\mathbf{f}}$ and $\mathbf{H}_{\boldsymbol{\sigma}} = \frac{\mathrm{d}\mathbf{h}}{\mathrm{d}\boldsymbol{\sigma}}$, $\boldsymbol{\sigma}_k \sim \mathrm{N}(0, \Sigma_k)$

A Unifying Perspective

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- For sequential data, the EKF / UKF / GHKF are equivalent to single-sweep EP where the moment matching is solved via linearisation.
- The iterated Kalman smoothers (EKS / UKS / GHKS) can also be recovered under certain parameter choices. But note that they optimise a different objective to EP (see paper for details).
- We show how natural gradient VI updates are surprisingly similar to the EP updates (when using a similar parametrisation).

New Algorithms

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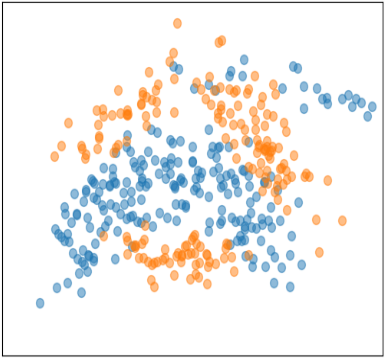
- We call this Extended Kalman Expectation Propagation (EK-EP).
- It has clear computational benefits when the parameter updates are high-dimensional, *e.g.*, in spatio-temporal problems.

Spatio-Temporal Classification

- We show that our smoothing methods can be applied to tasks with more than one input dimension.



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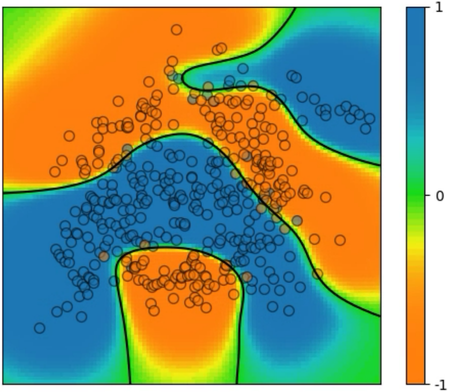

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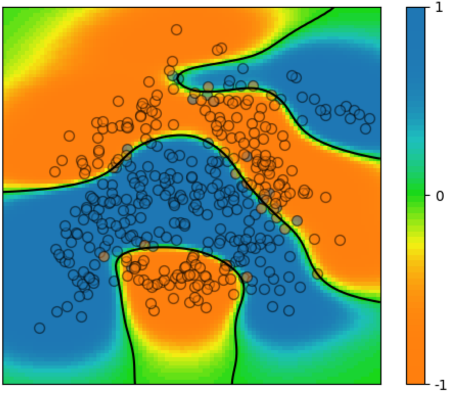

We treat the first dimension (x-axis) as time, and run iterated spatio-temporal smoothing (this demo uses EP).

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  iii) Exploits accelerated linear algebra (XLA) ops

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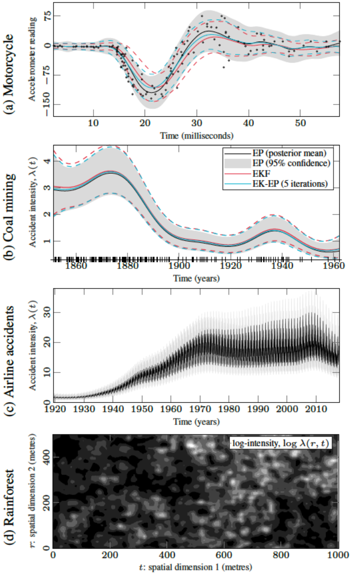
Results

We run extensive analysis on synthetic and real world data:

- Heteroscedastic Noise
- 1D & 2D Log Gaussian Cox Process
- 1D & 2D Classification
- Audio Amplitude Demodulation



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  - Sequential learning methods match the performance of batch methods, whilst scaling to larger data.
- See the paper for full results table.

Thanks for Listening

Take home messages:

- Any approximate inference method can be framed as a simple parameter update rule during Kalman smoothing.
- Sequential methods match the performance of batch methods, and can be extended to multiple dimensions.
- We provide fast JAX code for all methods.

Contact: `william.wilkinson@aalto.fi`

JAX code: `https://github.com/AaltoML/kalman-jax`