Challenges in building widely applicable GP software

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Stan

ArviZ

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  - GPs support is not a priority, but will get eventually better

Some applications

- predicting concrete quality
- spatial epidemiology
- cancer recurrence risk prediction
- finding minimum energy paths and saddle points
- ABC / likelihood free inference
- medicine dosage design

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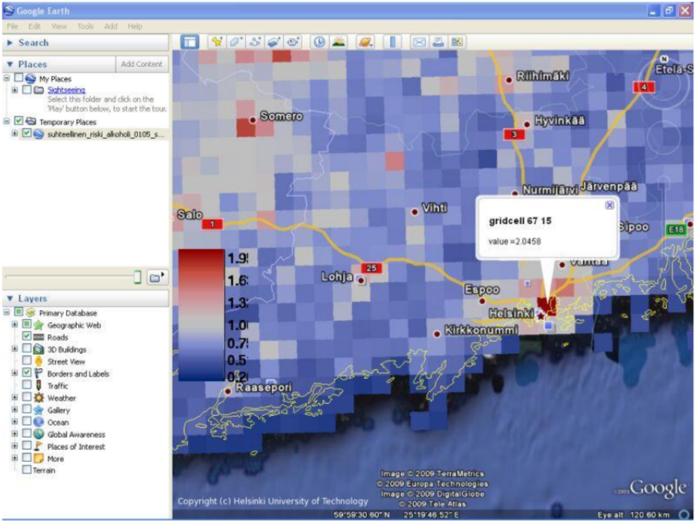

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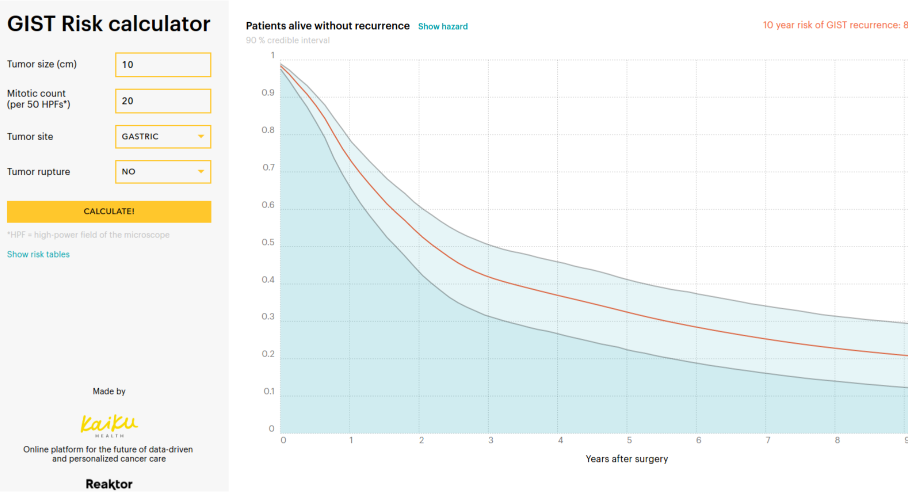

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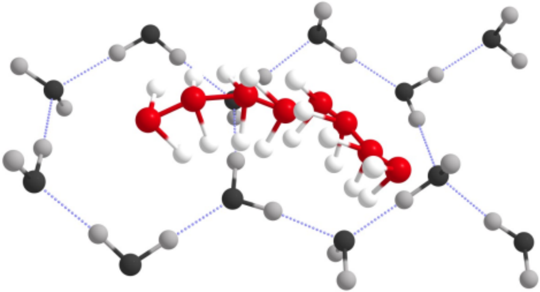

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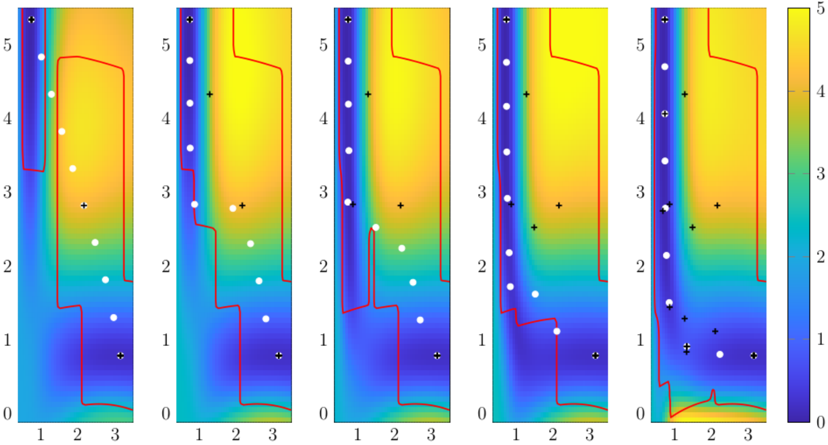

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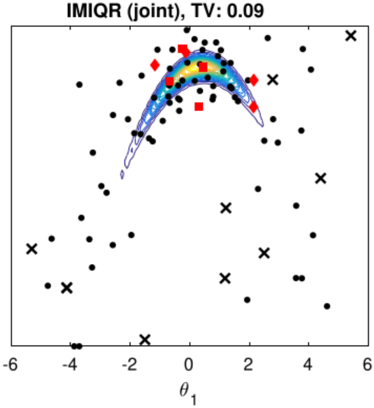

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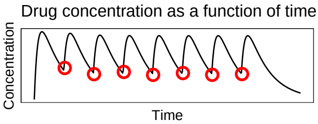

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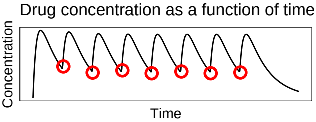
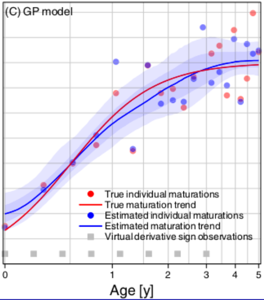


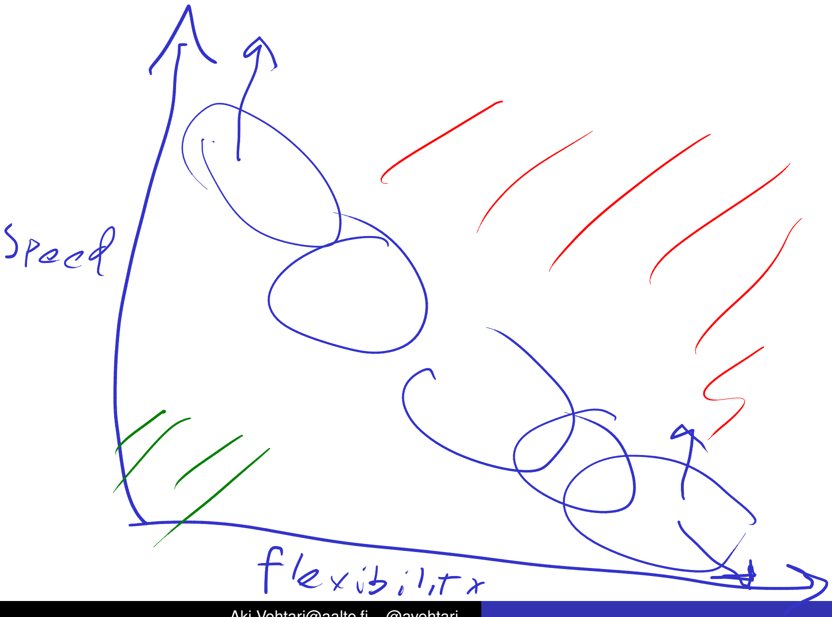


Some other software

- GPML
- GPy
- GPFlow
- GPtorch
- PyMC3
- TensorFlow probabilities
- Pyro
- Turing.JL
- INLA
- mgcv

https://en.wikipedia.org/wiki/Comparison_of_Gaussian_process_software

Flexibility vs speed



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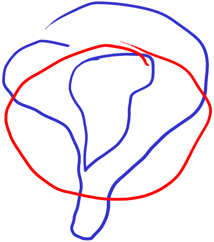
- Which approximation to use depends on e.g. stationarity, relative correlation length, combination of covariance functions

Speed

- The full joint posterior has difficult geometry
  - MCMC is likely to be slow
  - distributional approximations are likely to be bad
- The conditional distribution for latent values is easier
  - integrate out the latent variables using approximations
  - Laplace, EP, variational
  - if big data, maximizing marginal likelihood is ok
- Things get more difficult on the next slide

$$\underset{\sim}{f} \sim GP(0, K(x, x'; \hat{\underset{\sim}{\theta}}))$$

$$y \sim p(f, \hat{\underset{\sim}{\phi}})$$



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  - observation models depending on multiple latent values
  - observation models depending on multiple observations
  - censored data
  - multioutput
  - derivative observations

Flexibility vs complexity

- Combinatorial explosion if all features need to work together
  - approximate computation related to covariance matrix
  - approximate integration (latent or joint)
  - different observation models
  - different priors
  - combine with other models like ODEs

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- How about Turing complete probabilistic programming language, autodiff and automatic inference?
- Speed in autodiff systems is not automatic!
  - what is a node in autodiff?
  - forward, reverse, mixed, adjoints, etc.
- Inference speed depends on
  - computational cost of single (marginal) log density
  - difficult posterior geometries require more (marginal) log density evluations
  - integration vs maximzing marginal likelihood

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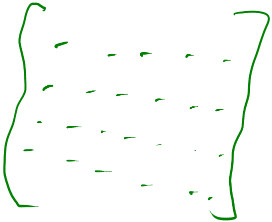
n^2

n^3



K[i,j] = a;

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- Even with these, Stan (or other generic PPL frameworks) is not competing with specialized software

Conclusion

- Very unlikely that one software would be best for everything
- Tradeoff between flexibility, speed, and additional implementation effort
- Prediction: There will be improvements in modularity and interoperability