

PROBABILISTIC NUMERICS IN 2023

Philipp Hennig

PN School – 27 March 2023



Tübingen AI Center
tuebingen.ai



Welcome!

The program

Monday		Tuesday		Wednesday	
9:00	Philipp Hennig	9:00	Tim Sullivan	9:00	Carl Henrik Ek
10:30	coffee	10:30	coffee	10:00	Fatemeh Yaghoobi
11:00	John Cunningham	11:00	Simo Särkkä	11:00	John Cockayne
12:00	Lunch	12:00	Lunch	12:00	Lunch
13:00		13:00		13:00	Masha Naslidnyk
14:00	Jonathan Wenger (P)	14:00	Nicholas Krämer	13:45	coffee
16:00	coffee	16:00	coffee	14:00	Toni Karvonen
16:30	Roman Garnett	16:30	Nathanael Bosch (P)	15:00	Emilia Magnani
		19:00	Dinner @ Freistil		

- ▶ dinner on Tuesday: for external participants only
- ▶ lunch/coffee: external participants take preference



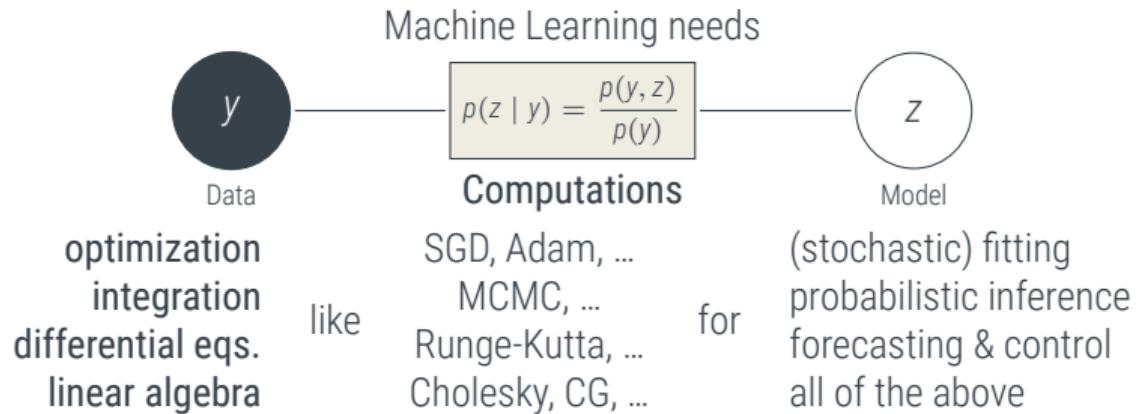
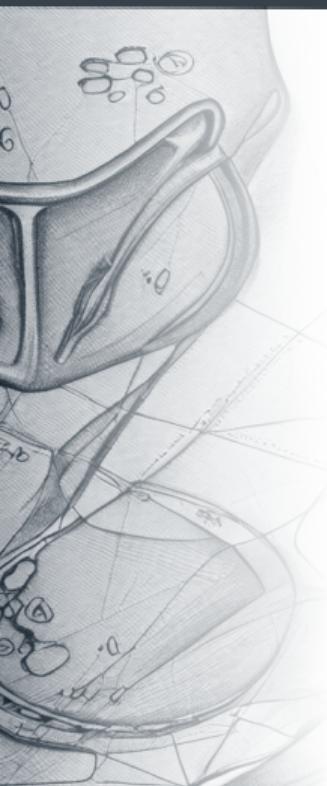
Probabilistic Numerics in 2023

Methods research just got even hotter



Machine Learning *is* Numerical Computation

Data from the disk: – contemporary AI methods require the solution of intractable mathematical tasks

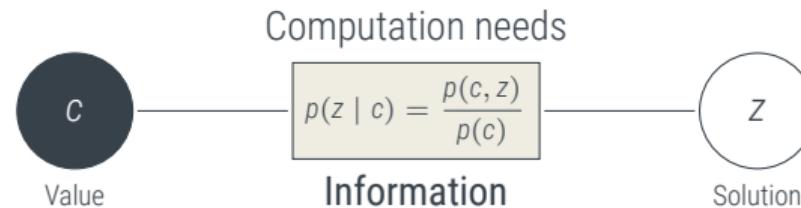
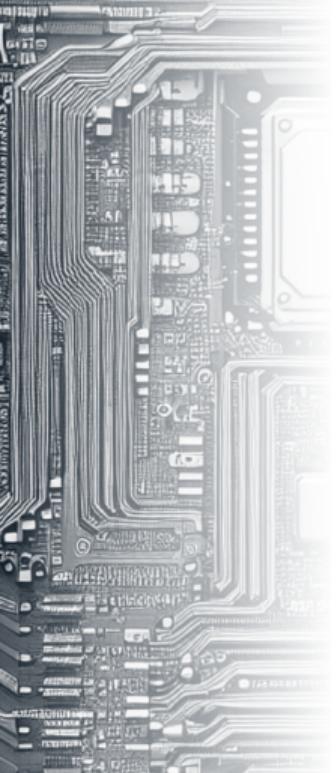


- ▶ classic (rule-based) AI required *analytic* computations (etc. nearest neighbors, shortest paths, etc.), modern AI/ML requires *numerical* methods
- ▶ **generic methods** save design time, but ML problems have idiosyncratic challenges ...



Numerical Computation *is* Machine Learning

Data from the chip: – a numerical method is an autonomous inference agent



optimization	estimate	$z = x \text{ s.t. } \nabla f(x) = 0$	given $\{c_i = \nabla f(x_i)\}$
integration	estimate	$z = \int_a^b f(x) dx$	given $\{c_i = f(x_i)\}$
simulation	estimate	$z = x(t) \text{ s.t. } x(t)' = f(x(t), t)$	given $\{c_i = f(x_i, t_i)\}$
linear algebra	estimate	$z = x \text{ s.t. } Ax = b$	given $\{As_i = c_i\}$

- ▶ A **probabilistic numerical method** produces a **probability measure** over the solution z to a non-analytic computational task, using tractable computations c as an **information sources**
- ▶ More details tomorrow in **Tim Sullivan's talk**



The native framework for AI/ML computation

What is Probabilistic Numerics?



A probabilistic numerical algorithm is a method that casts computation of intractable quantities in terms of (potentially approximate) probabilistic / Bayesian inference.

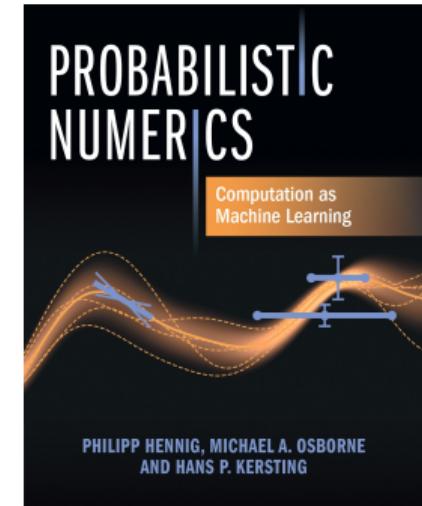
$$p(z | c) = \frac{p(c | z) \cdot p(z)}{p(c)}$$

Classics methods as special cases with $p(z) = \mathcal{GP}$, $p(c | z) = \delta(c - Az)$:

- ▶ Conjugate Gradients, Cholesky
- ▶ Runge-Kutta
- ▶ Gaussian quadrature
- ▶ Quasi-Newton (e.g. BFGS)

Advantages of probabilistic (re-) formulation include

- ▶ quantified, structured discretization uncertainty
- ▶ correct combination, and active control, of various computational and empirical information sources
- ▶ native description of imprecise computation through $p(c | z)$





Methods never mattered more

A research agenda for the generative AI age, and an outlook for the coming days

- ▶ mechanistic (simulation) and empirical (ML) information for scientific inference
- ▶ linear algebra for array-centric computation
- ▶ software engineering for deep learning



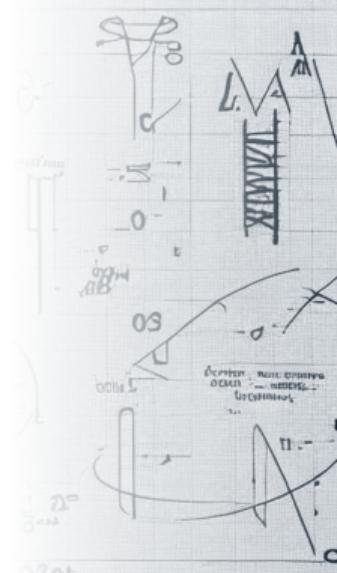


Assimilating information about dynamical systems

In science, good algorithms matter even more than anywhere else

- ▶ scientific inference might still be the most impactful domain for AI
- ▶ scientific questions often combine **sparse and expensive data** with generic but powerful mechanisms—laws of nature
- ▶ statistical inference is built to extract information from the data, **simulation methods** are built to extract information from the mechanism

Probabilistic simulation methods unite simulation and statistics, for information-agnostic inference on dynamical systems.

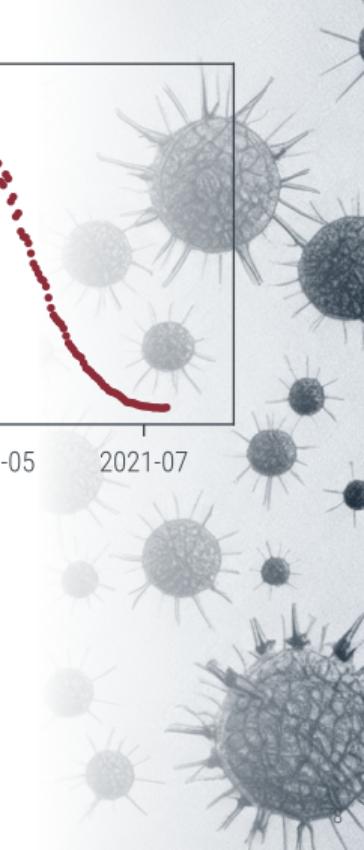
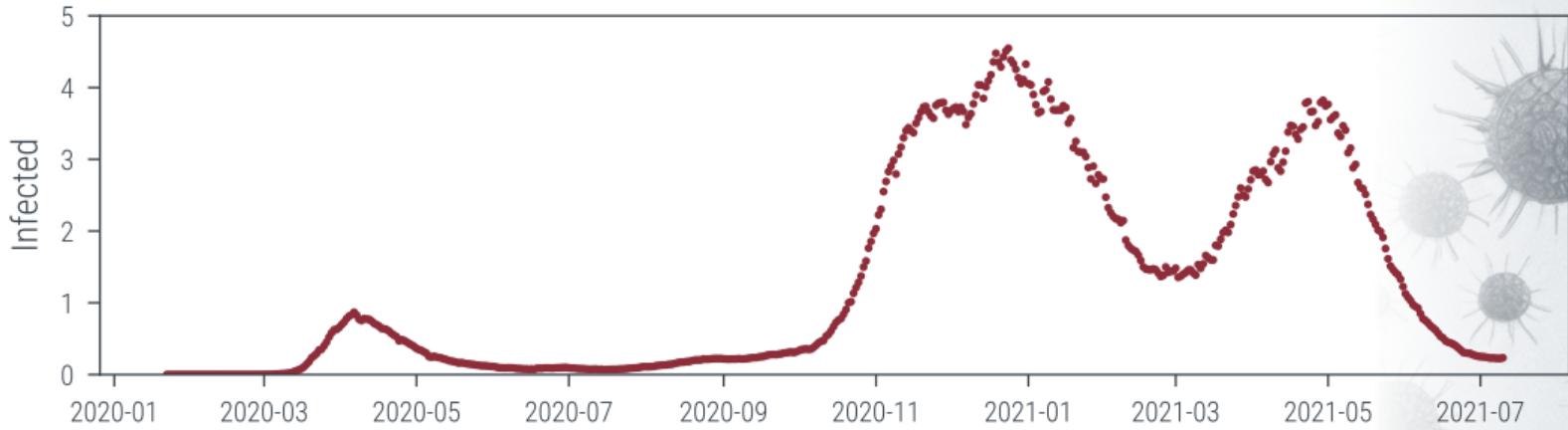




An inference problem, or a simulation problem?

Example: Pandemic modelling

Schmidt, Krämer, Hennig, 2021, NeurIPS 2021

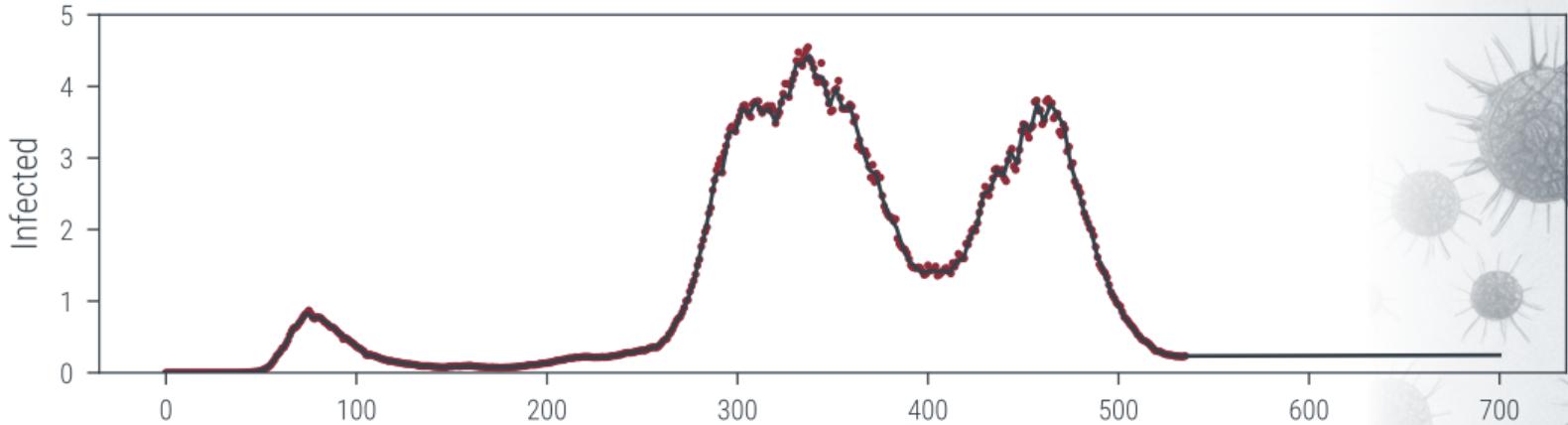




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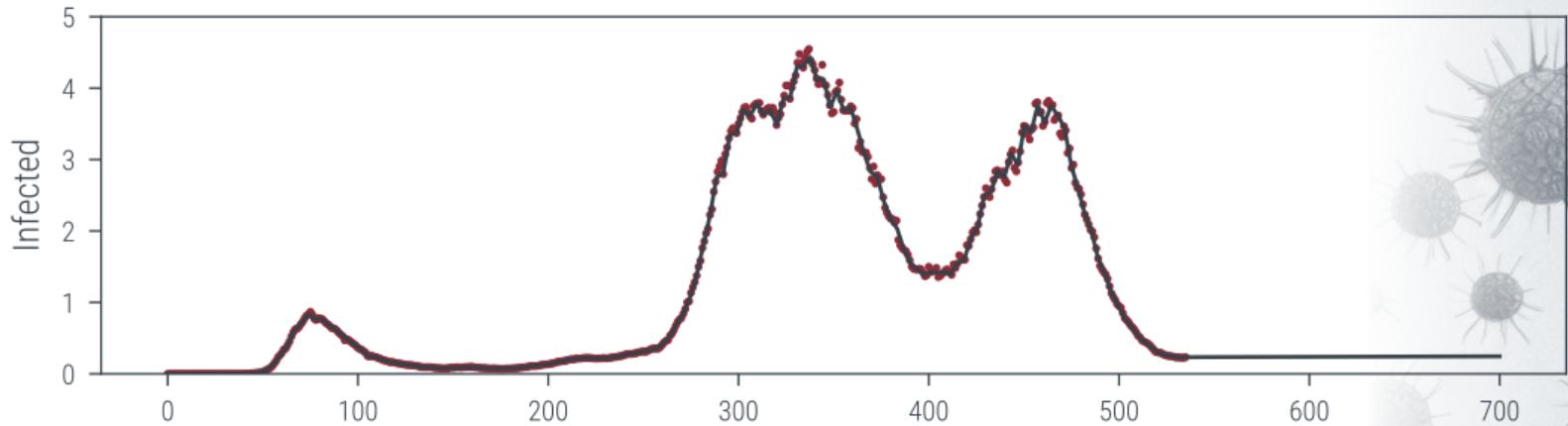




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Mechanistic knowledge encodes crucial scientific insight

$$\frac{d}{dt}x(t) = f(x(t), \beta(t))$$

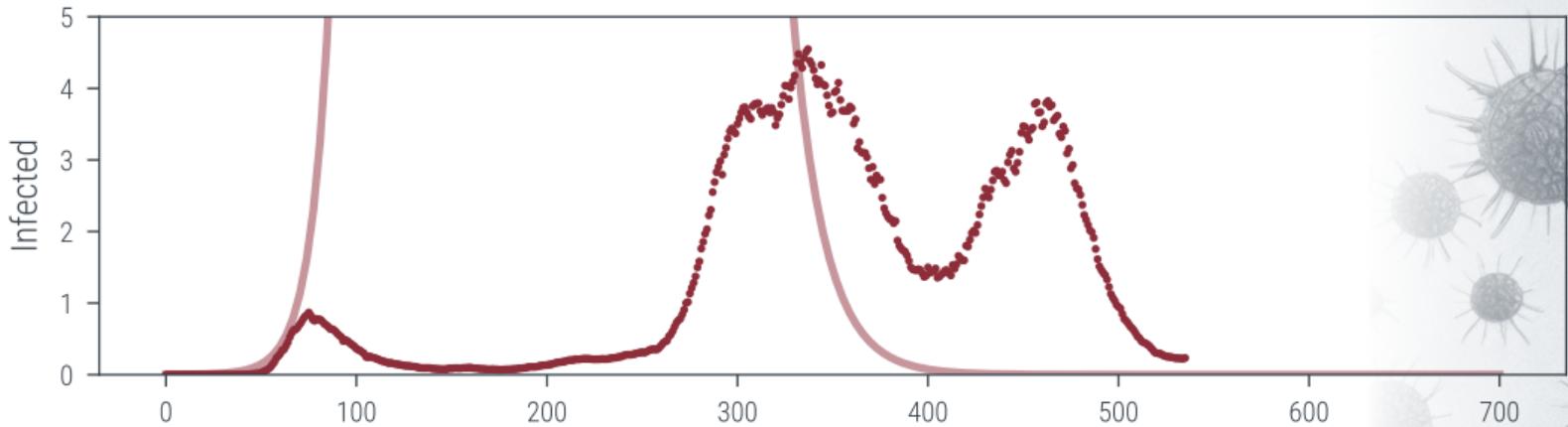
$$\frac{d}{dt} \begin{bmatrix} S(t) \\ I(t) \\ R(t) \end{bmatrix} = \begin{bmatrix} -\beta(t) \cdot S(t)I(t)/P \\ \beta(t) \cdot S(t)I(t)/P - \gamma I(t) \\ \gamma I(t) \end{bmatrix}$$



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But it requires *latent forces* that may be unknown



<https://github.com/scipy/scipy/blob/v1.9.1/scipy/integrate/dop/dopri5.f>

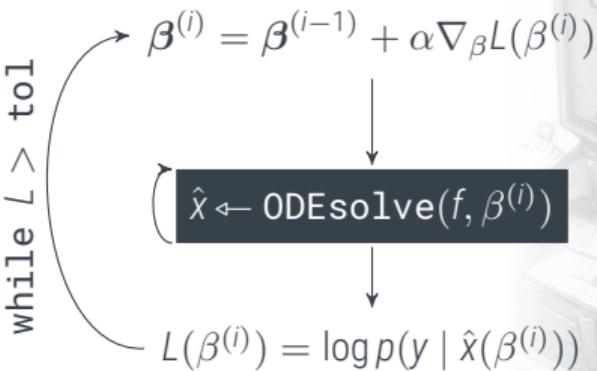
```
1      SUBROUTINE DOPRI5(N,FCN,X,Y,XEND,  
2      &                      RTOL,ATOL,ITOL,  
3      &                      SOLOUT,IOUT,  
4      &                      WORK,LWORK,IWORK,LIWORK,RPAR,IPAR,IDL)  
5 C -----  
6 C      NUMERICAL SOLUTION OF A SYSTEM OF FIRST ORDER  
7 C      ORDINARY DIFFERENTIAL EQUATIONS Y'=F(X,Y).  
8 C      THIS IS AN EXPLICIT RUNGE-KUTTA METHOD OF ORDER (4)5  
9 C      DUE TO DORMAND & PRINCE (WITH STEPSIZE CONTROL AND  
10 C     DENSE OUTPUT).  
11 C  
12 C     AUTHORS: E. HAIRER AND G. WANNER  
665    A51=19372.D0/6561.D0  
666    A52=-25360.D0/2187.D0  
667    A53=64448.D0/6561.D0  
668    A54=-212.D0/729.D0  
669    A61=9017.D0/3168.D0  
670    A62=-355.D0/33.D0
```

Inverse Problems can be solved with Backprop

automatic differentiation is amazing, but it does not answer scheduling of information

$$\frac{d}{dt} \begin{bmatrix} S(t) \\ I(t) \\ R(t) \end{bmatrix} = \begin{bmatrix} -\beta(t) \cdot S(t)I(t)/P \\ \beta(t) \cdot S(t)I(t)/P - \gamma I(t) \\ \gamma I(t) \end{bmatrix}$$

$$\frac{d}{dt} x = f(x(t), \beta(t))$$



- ▶ Define some loss $L(u)$, e.g.

$$L(u) := \sum_i -\log p(y_i | \hat{x}(u)) = \sum_i (y_i - H(\hat{x}(u)))^2 + \text{const.}$$

- ▶ Compute the gradient $\nabla_u L(u^{(i)})$ with automatic differentiation
- ▶ Example: [numppyro tutorial](#), using [jax's dopri5](#)
- ▶ Cf. *simulation-based inference (SBI)*, *approximate Bayesian computation (ABC)*, *Neural ODEs*, etc.

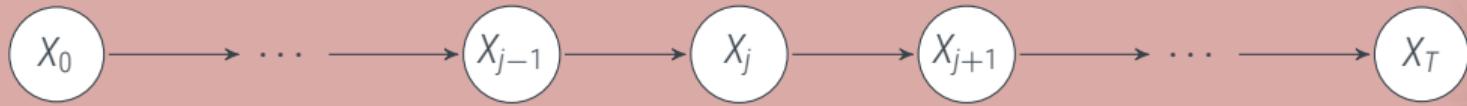


Simulation is inference from *information operators*

Bayesian filtering as a primitive for information assimilation

Tronarp, Kersting, Särkkä, Hennig, 2019

System State

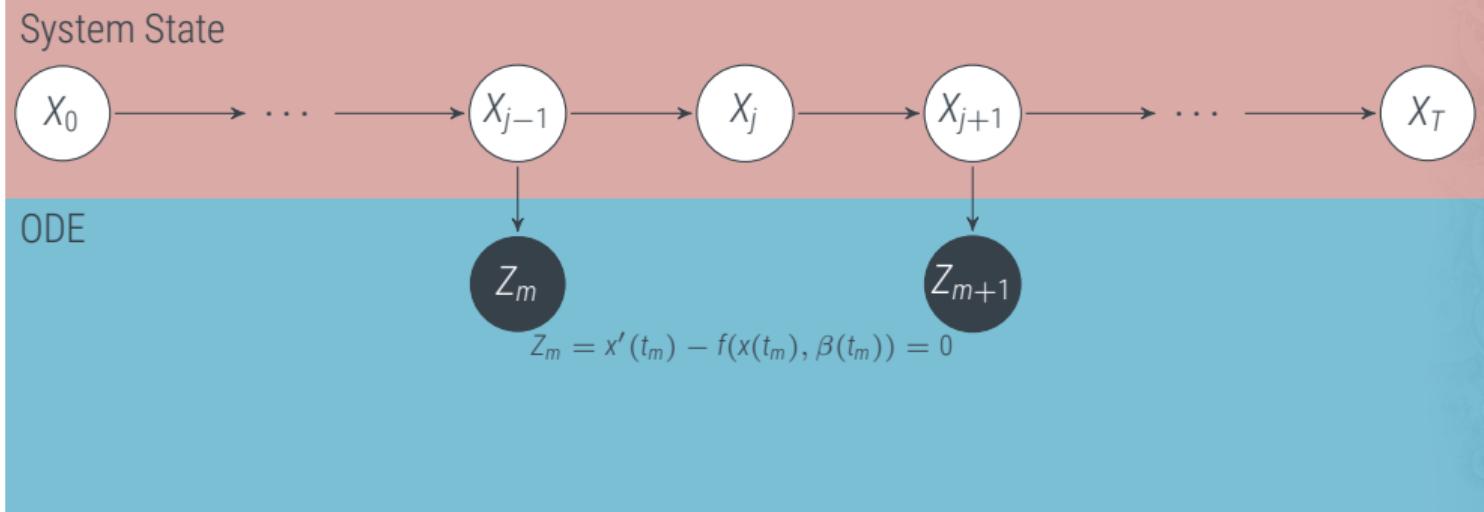




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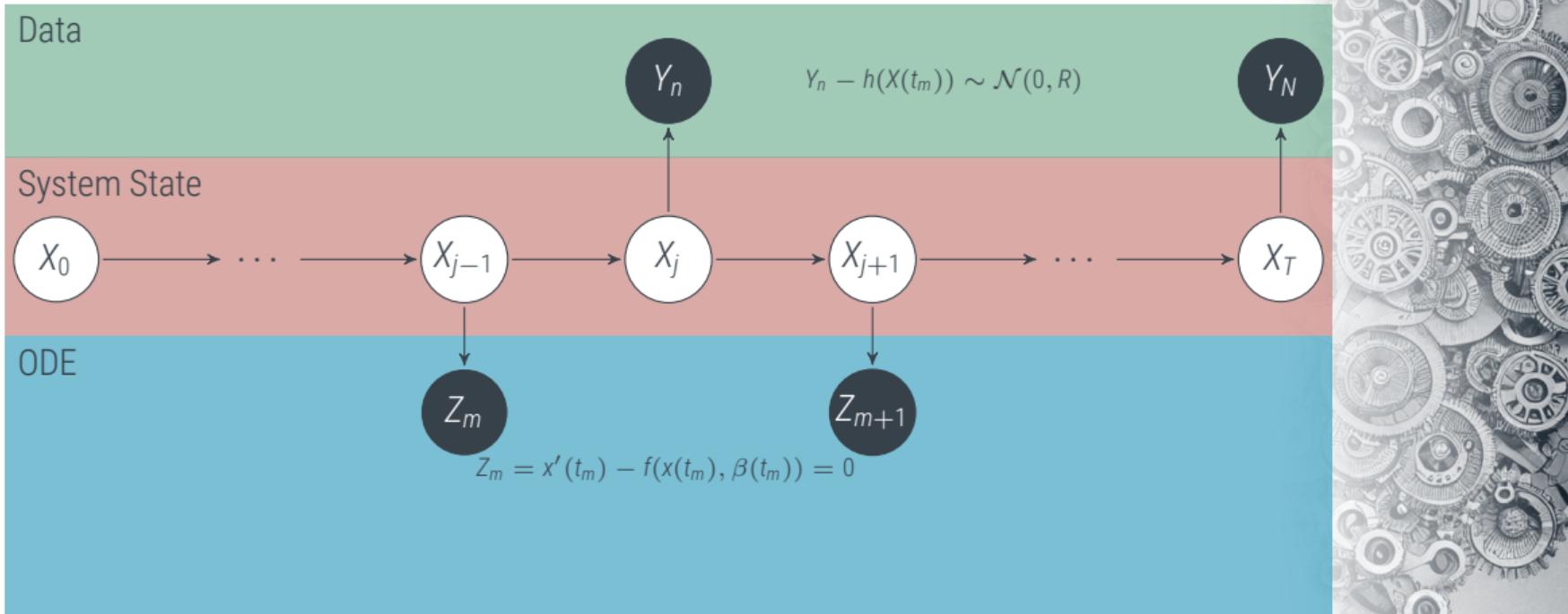




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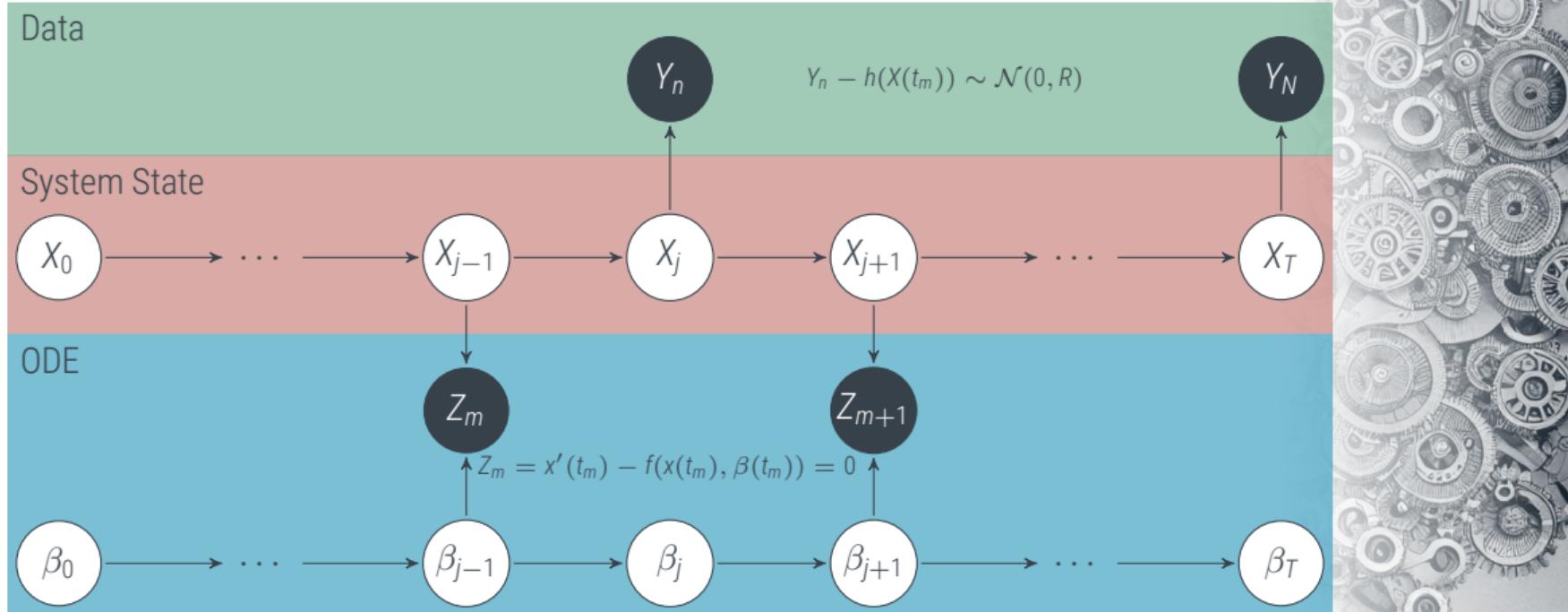




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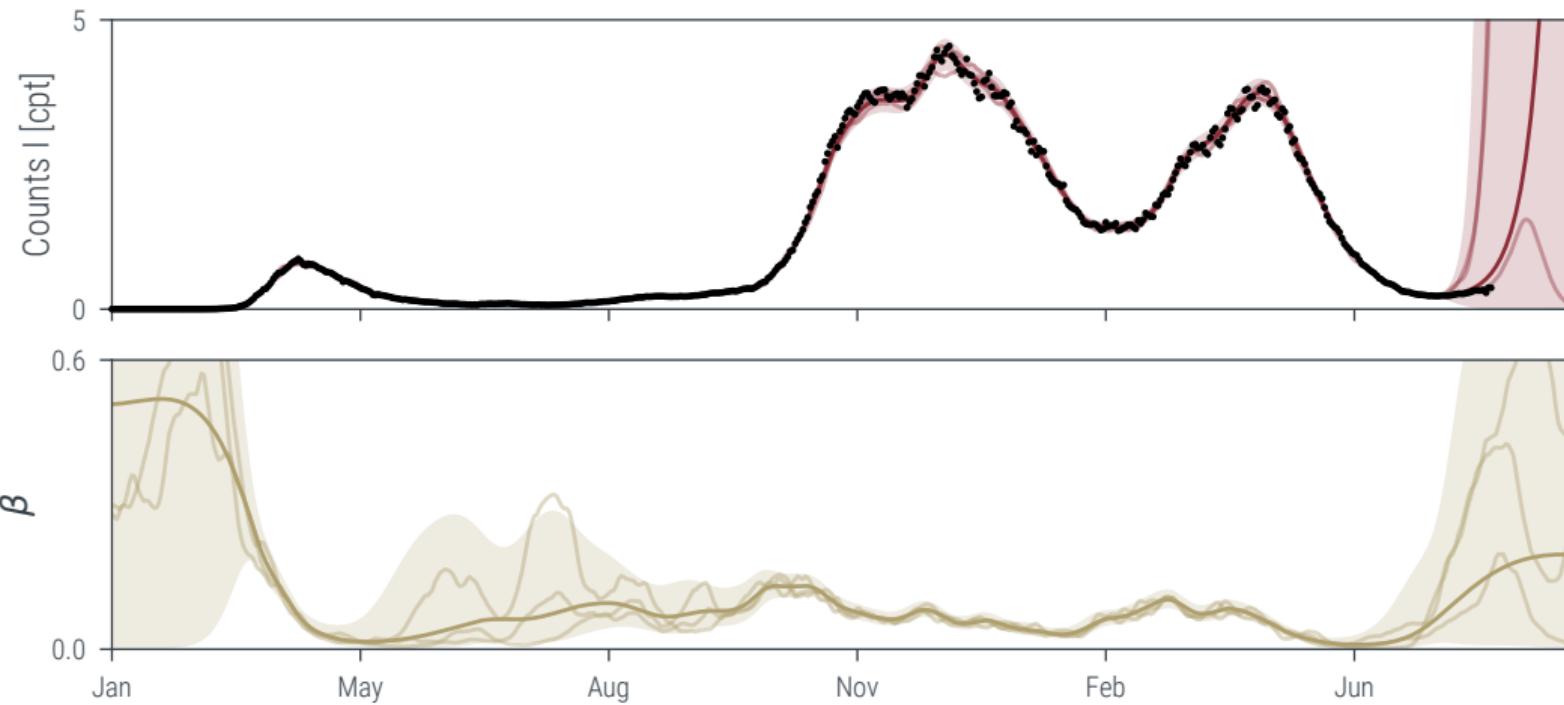
Bayesian filtering as a primitive for information assimilation

Tronarp, Kersting, Särkkä, Hennig, 2019



latent force and simulation in one pass

Example: Covid modelling





More about this *Tomorrow*

Keynotes and Tutorials on Time series and Simulation



Simo Särkkä
Tuesday, 11:00–12:30



Nicholas Krämer
Tuesday, 14:00–15:30



Nathanael Bosch
Tuesday, 16:30–18:00



Methods never mattered more

A research agenda for the generative AI age, and an outlook for the coming days

- ▶ mechanistic (simulation) and empirical (ML) information for scientific inference
- ▶ **Linear algebra for array-centric computation**
- ▶ software engineering for deep learning





How much does it cost to do GP inference?

more in today's keynotes / tutorials

$$G = k_{XX} + \sigma^2 I$$

$$\mu_\bullet = k_{\bullet X} \cdot \text{solve}(G, (y - \mu_X))$$

$$V_{\bullet\circ} = k_{\bullet X} - k_{\bullet X} \cdot \text{solve}(G, k_{X\circ})$$

Iterative linear solvers (even Cholesky) collect *projections* of G and y . **They are processing data from the disk iteratively.**

In linear algebra, **processing** and **loading** data are nearly the same thing. Thus, data is only really "there" once it has been computed on.

- ▶ read and process all data: $O(N^3)$
- ▶ construct and process k informative projections of G : $O(N^2k)$
- ▶ read and process k rows of G : $O(Nk^2)$
- ▶ read and process k random points, ignore rest: $O(k^3)$



Why do GPs still matter?

even in the age of LLMs, linear algebra won't die

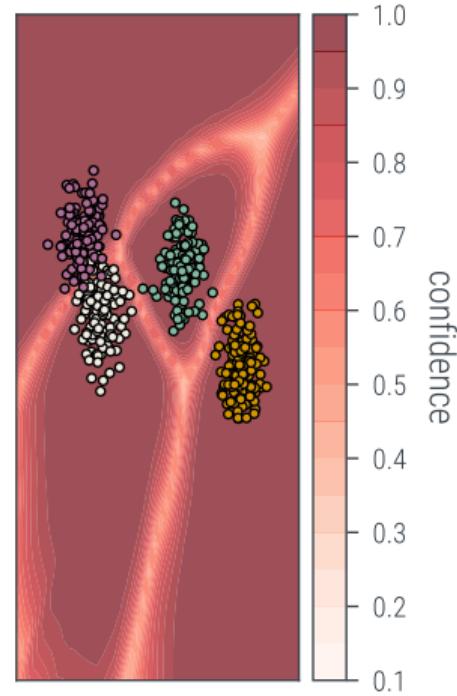
Khan et al. 2019, Kristiadi et al. 2020, 21, 22

Consider a deep network trained to find $\boldsymbol{\theta}_* \in \mathbb{R}^D$ as

$$\begin{aligned}\boldsymbol{\theta}_* &= \arg \min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) = \arg \min_{\boldsymbol{\theta}} \left(\frac{1}{N} \sum_{i=1}^N \underbrace{\ell(y_i; \widehat{f(x_i, \boldsymbol{\theta})})}_{\text{empirical risk}} + \underbrace{r(\boldsymbol{\theta})}_{\text{regularizer}} \right) \\ &= \arg \max_{\boldsymbol{\theta}} (\log p(\mathbf{y} | \boldsymbol{\theta}) + \log p(\boldsymbol{\theta})) = \arg \max_{\boldsymbol{\theta}} p(\boldsymbol{\theta} | \mathbf{y})\end{aligned}$$

Theorem: [Hein et al. 2019] If $f(x, \boldsymbol{\theta})$ is a ReLU network then, for almost any $x \in \mathbb{R}^d$ and $\varepsilon > 0$, there exists an $\alpha > 0$ and a class $k \in \{1, \dots, K\}$ such that for $z = \alpha x$

$$\frac{e^{f_k(x)}}{\sum_{r=1}^K e^{f_r(z)}} \geq 1 - \varepsilon \quad \text{and} \quad \lim_{\alpha \rightarrow \infty} \frac{e^{f_k(\alpha x)}}{\sum_{r=1}^K e^{f_r(\alpha x)}} = 1$$





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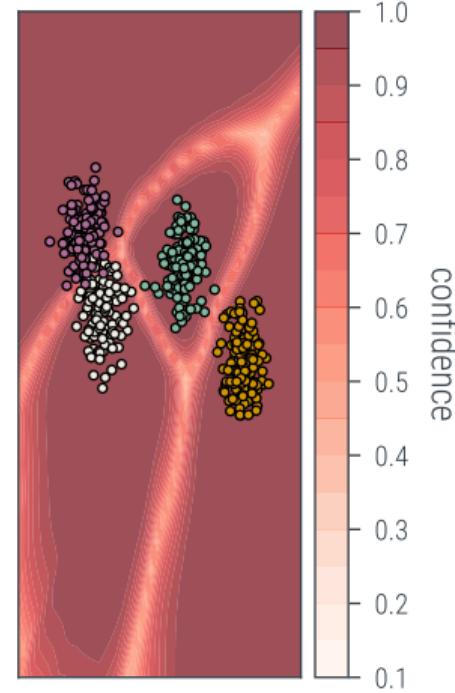
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find the Laplace approximation, with $[\Psi(\boldsymbol{\theta})]_{ij} = \frac{\partial \mathcal{L}(\boldsymbol{\theta})}{\partial \theta_i \partial \theta_j}$

$$\mathcal{L}(\boldsymbol{\theta}) = \mathcal{L}(\boldsymbol{\theta}_*) + 1/2(\boldsymbol{\theta} - \boldsymbol{\theta}_*)^\top \Psi(\boldsymbol{\theta}_*)(\boldsymbol{\theta} - \boldsymbol{\theta}_*)$$

$$p(\boldsymbol{\theta} | \mathbf{x}, \mathbf{y}) \approx \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\theta}_*, -\Psi^{-1})$$

This requires numerical linear algebra!



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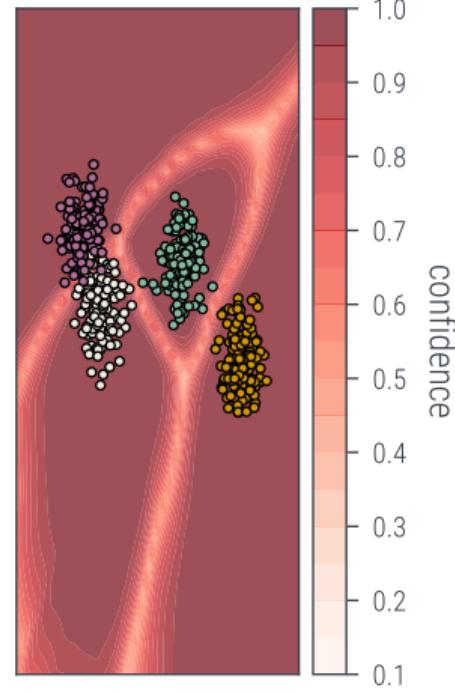
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linearization $f(\mathbf{x}, \boldsymbol{\theta}) = f(\mathbf{x}, \boldsymbol{\theta}_*) + J(\mathbf{x}, \boldsymbol{\theta}_*)(\boldsymbol{\theta} - \boldsymbol{\theta}_*)$, using $[J]_{ij} = \frac{\partial f_i(\mathbf{x}, \boldsymbol{\theta})}{\partial \theta_j}$

$$p(f(\mathbf{x}) | \mathbf{x}, \mathbf{y}) = \int p(f(\mathbf{x}, \boldsymbol{\theta}) | \mathbf{x}, \mathbf{y}) p(\boldsymbol{\theta}) d\boldsymbol{\theta} \approx \mathcal{GP}(f; f(\mathbf{x}, \boldsymbol{\theta}_*), -J(\mathbf{x}) \Psi^{-1} J(\mathbf{x})^\top)$$



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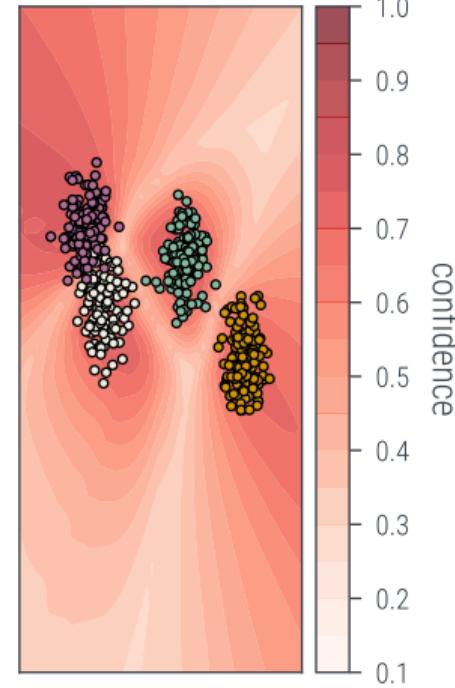
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More about GPs Today

Keynotes and Tutorials on linear Gaussian inference and Bayesian optimization



John Cunningham
Monday, 11:00–12:30



Johnathan Wenger
Monday, 14:00–15:30



Roman Garnett
Monday, 16:00–17:30



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- ▶ **software engineering for deep learning**

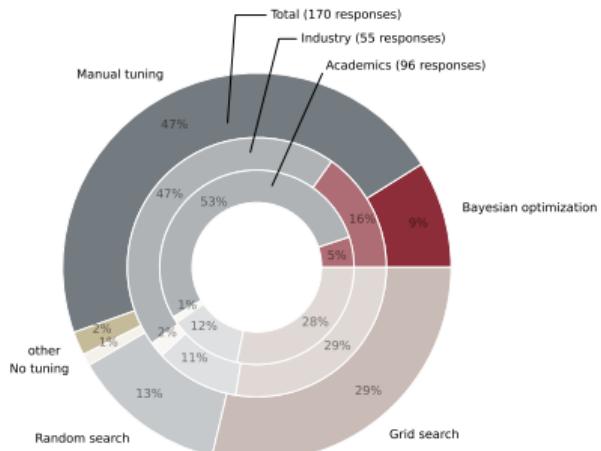


Deep Training is not Mature

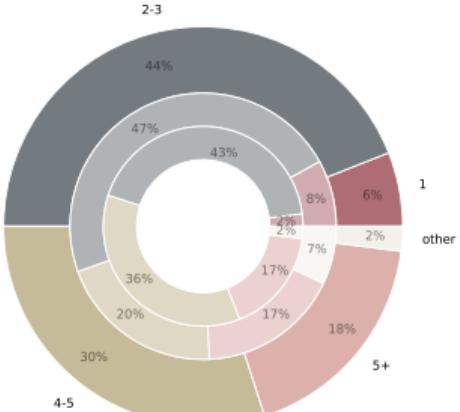
Results of a NeurIPS workshop 2023



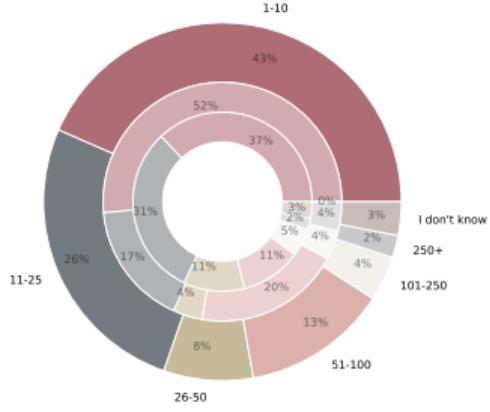
How do you tune your training?



How many parameters do you tune?



How many tuning trials do you need?



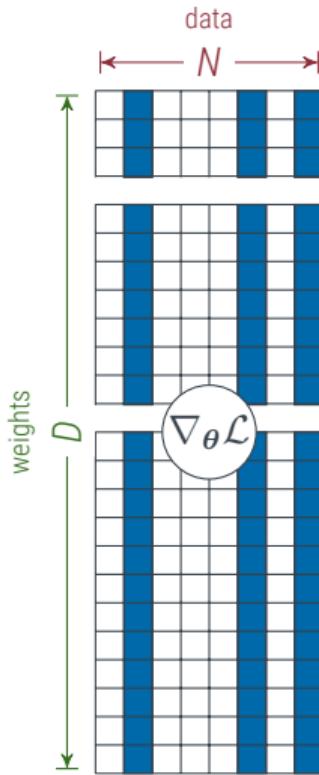
- ▶ In deep learning, computation is often an experiment to collect data
- ▶ more on automating this process in **Roman Garnett's talk**





Array-centric Programming

The deep learning software stack is not yet mature



$$\boldsymbol{\theta}_* = \arg \min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) = \arg \min_{\boldsymbol{\theta}} \left(\frac{1}{N} \sum_{i=1}^N \ell(y_i; f(x_i, \boldsymbol{\theta})) + r(\boldsymbol{\theta}) \right)$$

auto-diff and batching ($N \ll M$)

$$\begin{aligned} \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{\theta}) &= \frac{1}{N} \sum_{i=1}^N \nabla_{\boldsymbol{\theta}} \ell(y_i; f(x_i, \boldsymbol{\theta})) + \nabla_{\boldsymbol{\theta}} r(\boldsymbol{\theta}) \\ &\approx \frac{1}{M} \sum_{j=1}^M \nabla_{\boldsymbol{\theta}} \ell(y_j; f(x_j, \boldsymbol{\theta})) + \nabla_{\boldsymbol{\theta}} r(\boldsymbol{\theta}) =: g(\boldsymbol{\theta}) \end{aligned}$$

yield a random variable

$$p(g(\boldsymbol{\theta}) \mid \nabla_{\boldsymbol{\theta}} \mathcal{L}) \approx \mathcal{N} \left(g(\boldsymbol{\theta}); \nabla_{\boldsymbol{\theta}} \mathcal{L}, \Sigma \in \mathcal{O} \left(\frac{N-M}{NM} \right) \right)$$



Computing statistics is not expensive

contemporary differentiable programming frameworks constrain users

Dangel, Künstner, PH, ICLR 2020, <https://backpack.pt>

$$\nabla \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^N \nabla \ell(y_i; \boldsymbol{\theta}) \approx \frac{1}{M} \sum_{j=1}^M \nabla \ell(y_j; \boldsymbol{\theta}) =: g(\boldsymbol{\theta}) \quad \text{already computed!}$$

```
1 from torch.nn import CrossEntropyLoss, Linear
2
3 X, y = load_data()
4 model = Linear(784, 10)
5 lossfunc = CrossEntropyLoss()
6 loss = lossfunc(model(X), y)
7 loss.backward()
8
9 for param in model.parameters():
10     print(param.grad) # this is g(theta). Where is Sigma?
```



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$$\nabla \mathcal{L}(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^N \nabla \ell(y_i; \boldsymbol{\theta}) \approx \frac{1}{M} \sum_{j=1}^M \nabla \ell(y_j; \boldsymbol{\theta}) =: g(\boldsymbol{\theta}) \quad \text{already computed!}$$

$$\sigma^2(\boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^N [\nabla \ell(y_i; \boldsymbol{\theta})]^2 \approx \frac{1}{M} \sum_{j=1}^M [\nabla \ell(y_j; \boldsymbol{\theta})]^2 =: \hat{\sigma}^2(\boldsymbol{\theta}) \quad \text{variance adds minimal overhead}$$

```
1 # pip install backpack-for-pytorch
2 from backpack import extend, backpack, Variance
3
4 model = extend(Linear(784, 10))
5 lossfunc = extend(CrossEntropyLoss())
6 loss = lossfunc(model(X), y)
7
8 with backpack(Variance()):
9     loss.backward()
10
11 for param in model.parameters():
12     print(param.grad) # this is g(theta). Where is sigma2?
13     print(param.variance) # here it is!
```



Probabilistic quantities are accessible

pip install backpack-for-pytorch and <https://backpack.pt>

Dangel, Künstner, Hennig, ICLR 2020

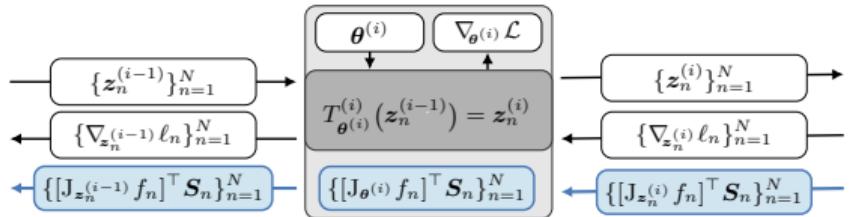
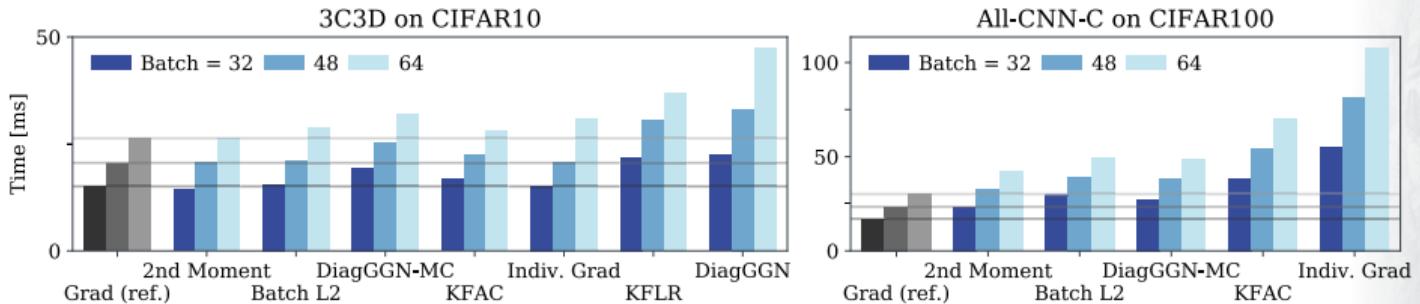


Figure 5: Schematic of the additional backward pass to compute a symmetric factorization of the GGN,
 $G(\theta) = \sum_n [J_\theta f_n]^\top S_n S_n^\top [J_\theta f_n]$
alongside the gradient at the i th module, for N samples.



Probabilistic Software Engineering

pip install cockpit-for-pytorch





- ▶ As AI/ML goes through the generative revolution, **algorithms** only get *more* relevant
- ▶ features of advanced ML, like
 - ▶ mix of mechanistic and empirical knowledge
 - ▶ computation as experimentation
 - ▶ batched array processing
- ▶ blur the line between information *collection* and information *processing*, information *from the disk* and *from the chip*
- ▶ Probabilistic Numerics provides a common, native language for information management in AI systems
- ▶ let us build the probabilistic ML stack together!

Join the Competition

The MLCommons AlgoPerf challenge



- ▶ A competition between algorithms for neural network training speed
- ▶ Algorithmic Performance challenge to be released soon
- ▶ separate rule-set for self-tuning algorithms
- ▶ a two year effort by 25+ scientists from Google, Tübingen, Meta, Toronto and others
- ▶ find out more from Frank Schneider

ML
● Commons

