lsbi: linear simulation based inference

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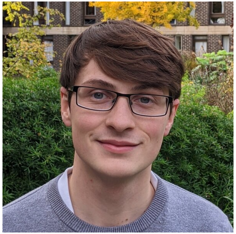
Context from phystat

- From **Jesse Thaler**'s talk on Interpretable Machine Learning:
  "If asked what is the most under-used Machine Learning technique in physics...
  ... my answer is only half-jokingly **linear regression***."*
- sbi mentioned in (so far)
  - Monday
    - Ben Wandelt Cosmology and machine learning¶
    - Maximilian Dax Simulation-based machine learning for gravitational-wave analysis
    - Andre Scaffidi Anomaly aware machine learning for dark matter direct detection at the DARWIN experiment
    - Joshua Villarrea Feldman-Cousins' ML Cousin
  - Tuesday
    - Aishik Ghosh Simulation-based Inference (SBI)

Who?



Idea I've been working on/talking about for the better part of 18 months,

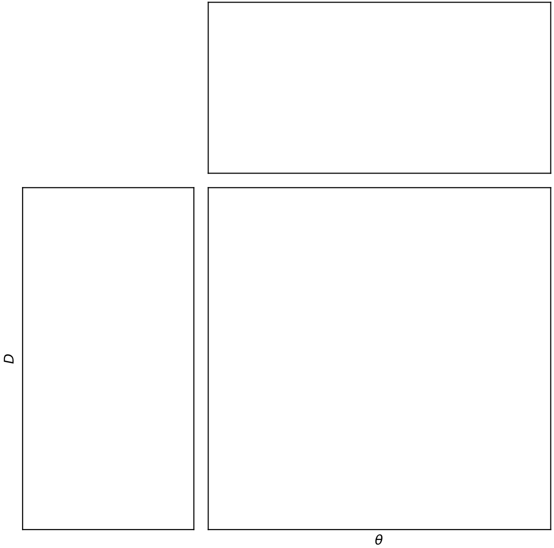
- Nicolas Mediato Diaz (MSci project)
- David Yallup (Postdoc)
- Thomas Gessey Jones (Postdoc)

Many others have also presented this idea independently

- `SELFI` incorporates much of this idea: Leclercq [1902.10149]
- some of these ideas are in `MOPED`: Heavens [astro-ph/9911102]
- Also appears in Häggström [2403.07454]

SBI: Simulation-based inference

- What do you do if you don't know $\mathcal{L}(D|\theta)$?
- If you have a simulator/forward model $\theta \rightarrow D$ defines an *implicit* likelihood $\mathcal{L}$.
- Simulator generates samples from $\mathcal{L}(\cdot|\theta)$.
- With a prior $\pi(\theta)$ can generate samples from joint distribution $\mathcal{J}(\theta, D) = \mathcal{L}(D|\theta)\pi(\theta)$ *the "probability of everything"*.
- Task of SBI is take joint $\mathcal{J}$ samples and learn posterior $\mathcal{P}(\theta|D)$, and evidence $\mathcal{Z}(D)$ or even likelihood $\mathcal{L}(D|\theta)$ or joint $\mathcal{J}(\theta, D)$.
- Present state of the art achieves this using *machine learning* (neural networks).



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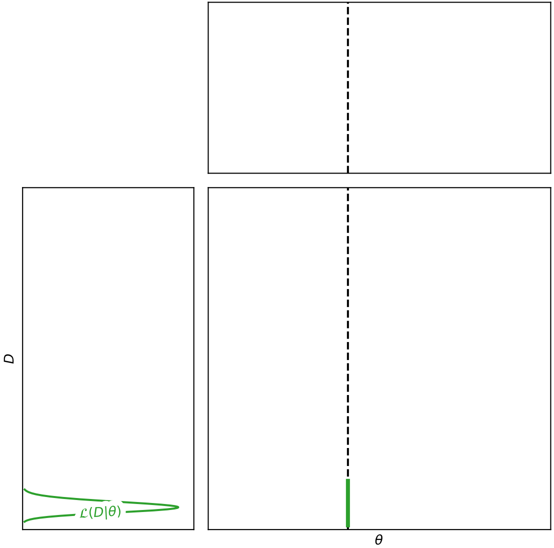

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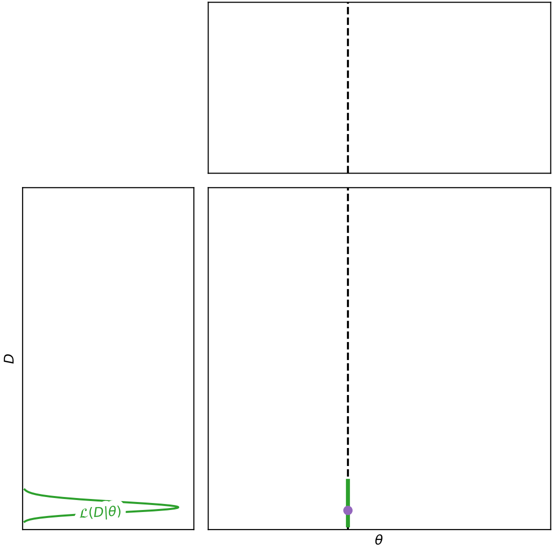

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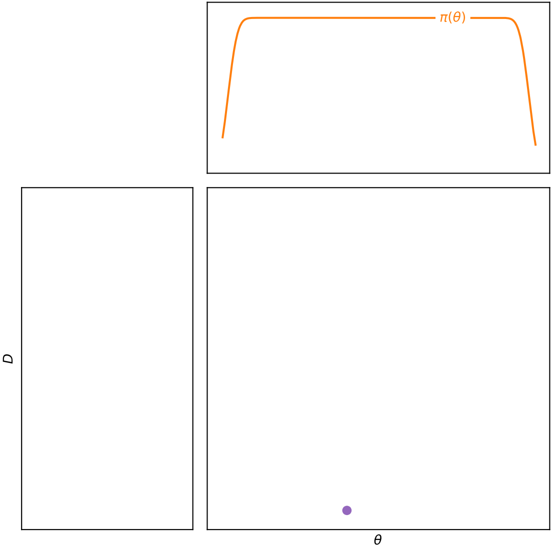

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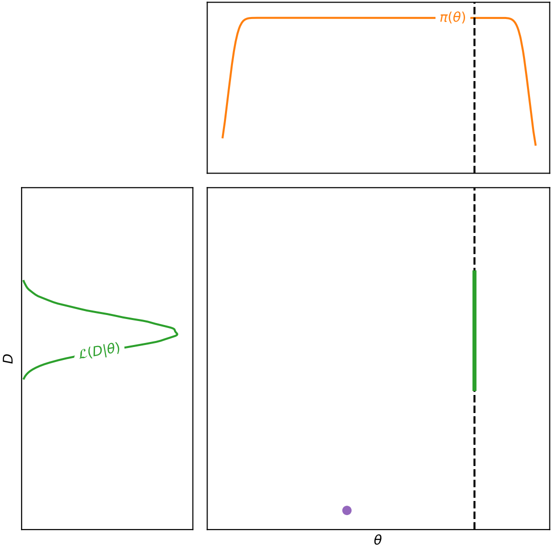

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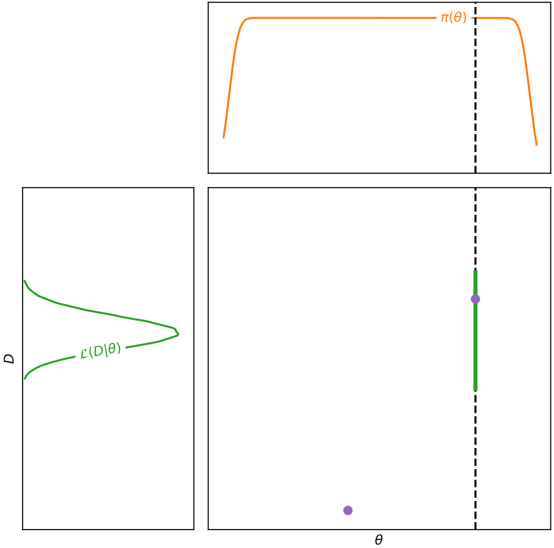

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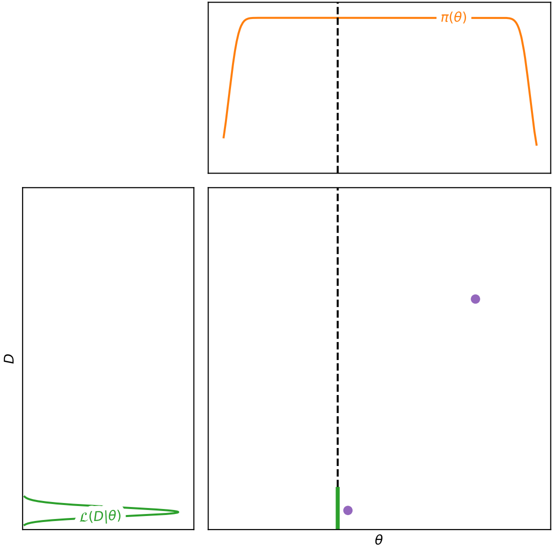

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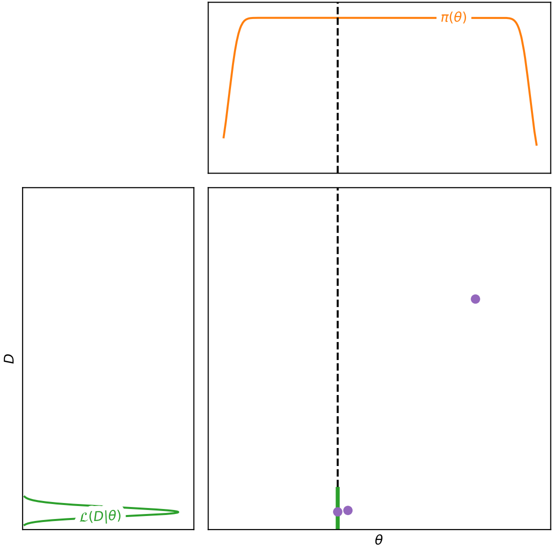

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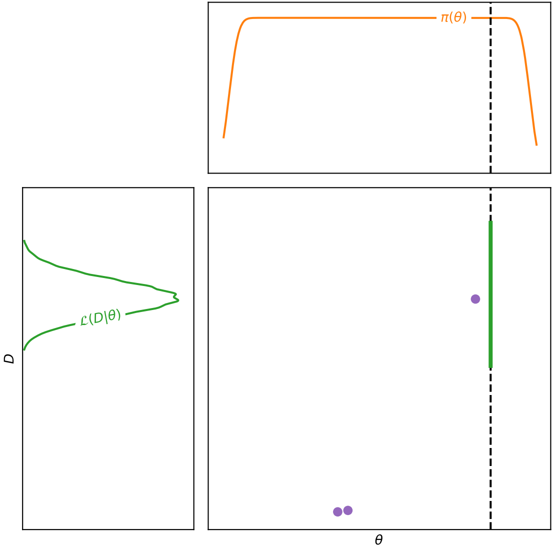

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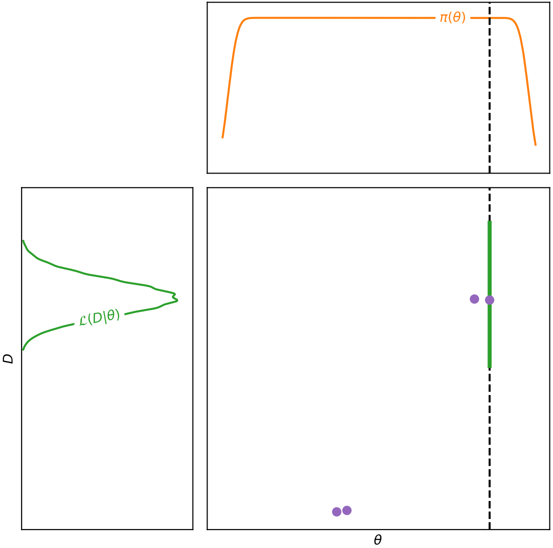

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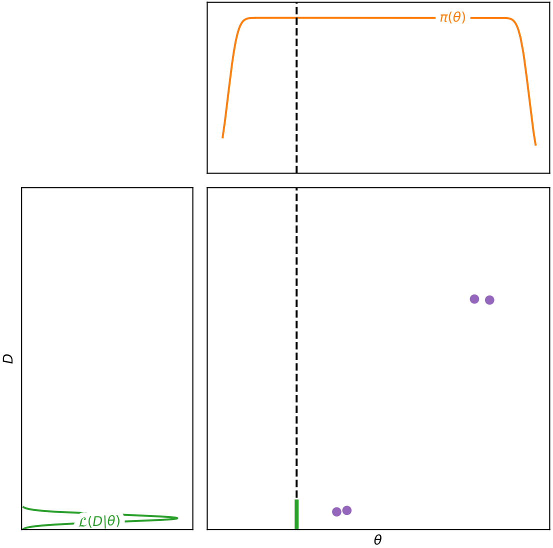

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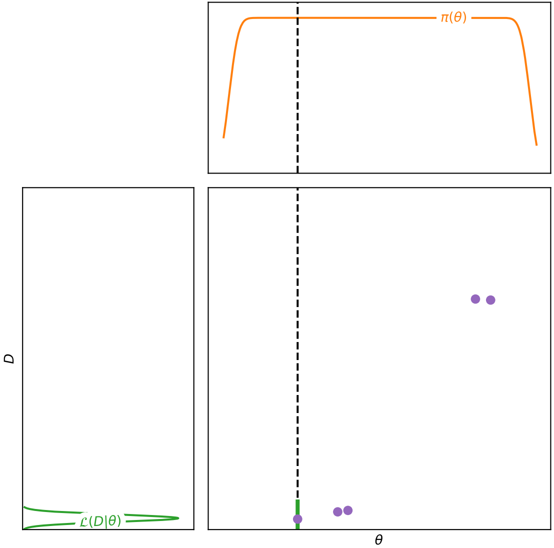

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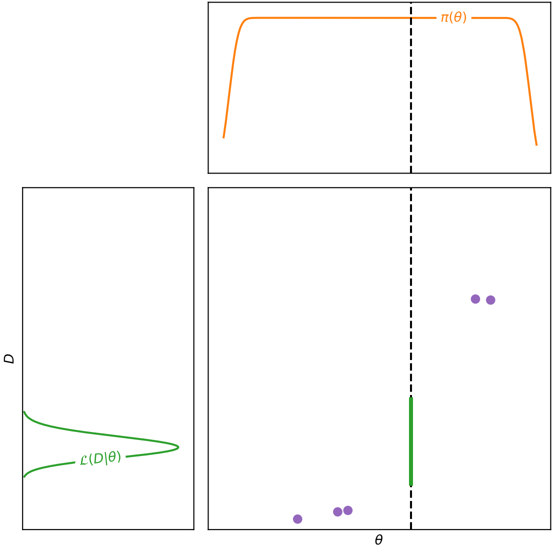

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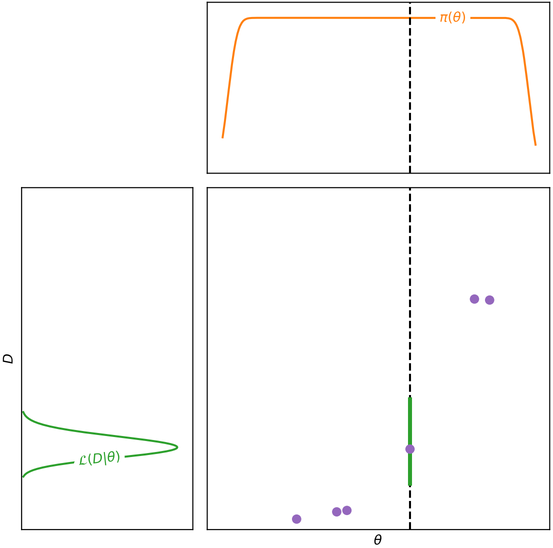

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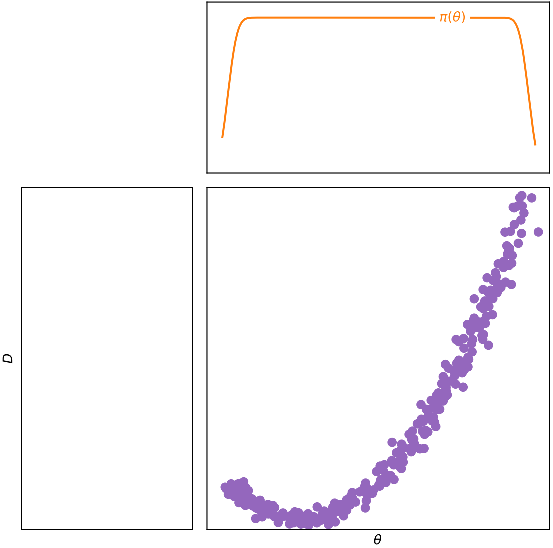

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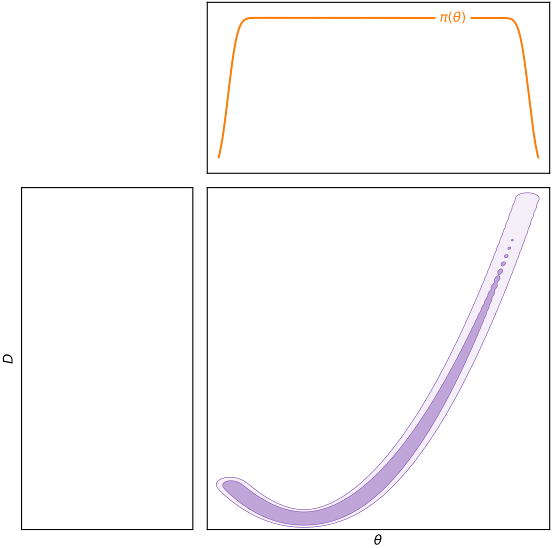

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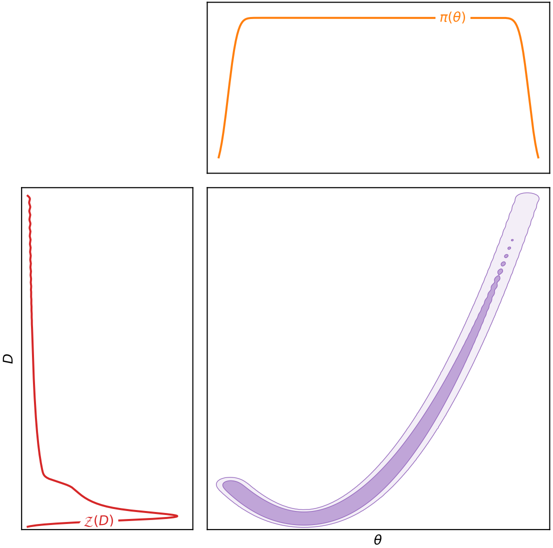

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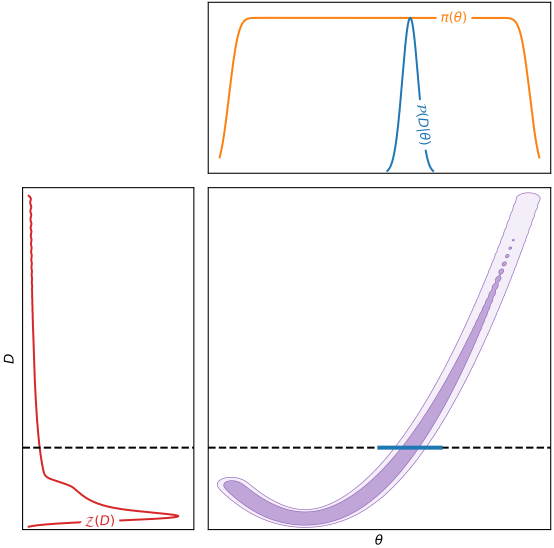

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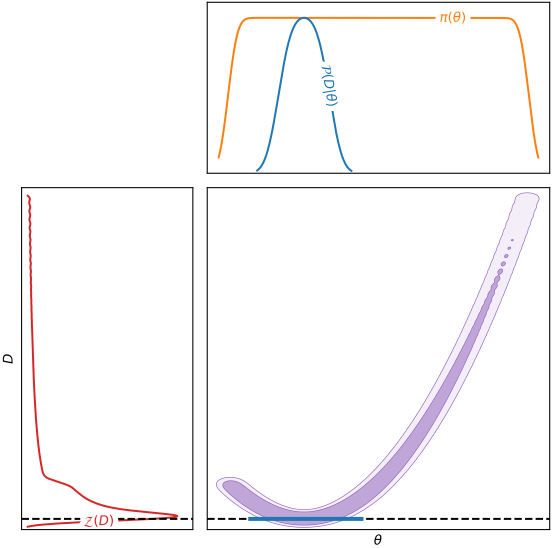

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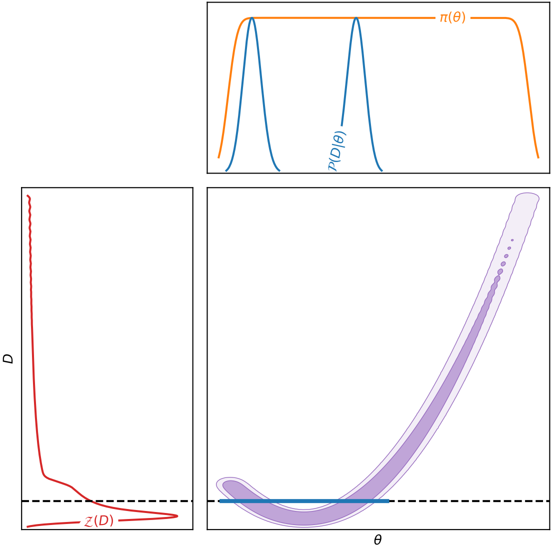

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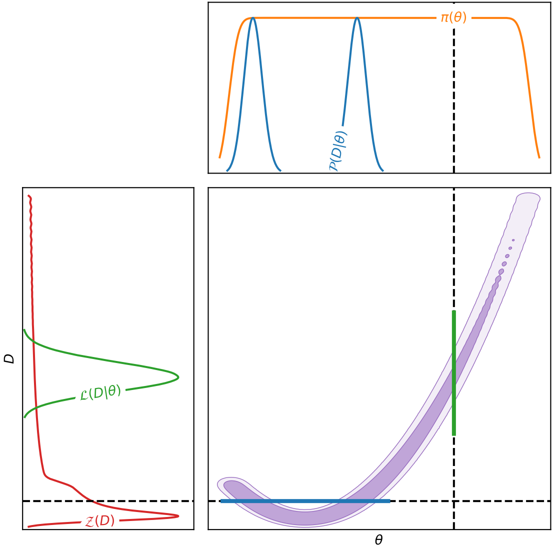

Why linear SBI?

If neural networks are all that, why should we consider the regressive step of going back to linear versions of this problem?

- It is pedagogically helpful
  - separates general principles of SBI from the details of neural networks
  - (particularly for ML skeptics)
- It is practically useful
  - for producing expressive examples with known ground truths.
- It is pragmatically useful
  - competitive with neural approaches in terms of accuracy,
  - faster and more interpretable.

- Linear generative model (m, M, C)

$$D = m + M\theta \pm \sqrt{C}$$

where:

$$\begin{aligned} \theta &: n \text{ dimensional parameters} \\ D &: d \text{ dimensional data} \\ M &: d \times n \text{ transfer matrix} \\ m &: d\text{-dimensional shift} \\ C &: d \times d \text{ data covariance} \end{aligned}$$

[1]N.B. using matrix variate notation where primes denote transposes $M' = M^T$

Linear Simulation Based Inference

Mathematical setup

- Linear generative model (m, M, C)

$$D \sim \mathcal{N}(m + M\theta, C)$$

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- k Simulations

$$S = \{(\theta_i, D_i) : i = 1, \ldots, k\}$$

- Define simulation statistics[1]:

$$\begin{aligned} \bar{\theta} &= \tfrac{1}{k}\textstyle\sum_k \theta_i \\ \bar{D} &= \tfrac{1}{k}\textstyle\sum_k D_i \\ \Theta &= \tfrac{1}{k-1}\textstyle\sum_i (\theta_i - \bar{\theta})(\theta_i - \bar{\theta})' \\ \Delta &= \tfrac{1}{k-1}\textstyle\sum_i (D_i - \bar{D})(D_i - \bar{D})' \\ \Psi &= \tfrac{1}{k-1}\textstyle\sum_i (D_i - \bar{D})(\theta_i - \bar{\theta})' \end{aligned}$$

[1] N.B. using matrix variate notation where primes denote transposes $M' = M^T$

Linear Simulation Based Inference: gory mathematical details

- We now wish to infer the parameters of the linear model (m, M, C) from simulations S (which define $\bar\theta, \bar D, \Theta, \Delta, \Psi$)
- The likelihood for this problem is:

$$P(\{D_i\}|\{\theta_i\}|m, M, C) = \prod_i \mathcal{N}(D_i|m + M\theta_i, C)$$

- It can be shown the posterior $\mathcal{P}$ is...

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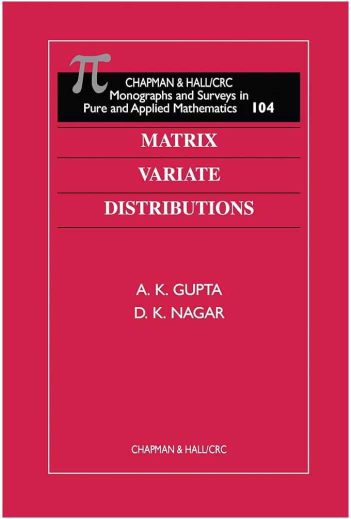

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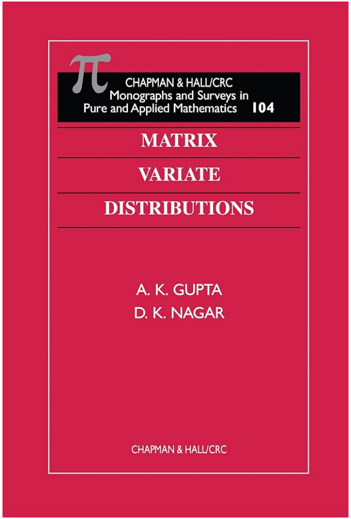
$$m|M, C, S \sim \mathcal{N}\left(\tfrac{k}{k+1}(\bar D - M\bar\theta), \tfrac{C}{k+1}\right),$$
$$M|C, S \sim \mathcal{MN}\left(\Psi\Theta_*^{-1}, \tfrac{C}{k-1}, \Theta_*^{-1}\right),$$
$$C|S \sim \mathcal{W}_\nu^{-1}\left(C_0 + (k-1)(\Delta - \Psi\Theta^{-1}\Psi')\right),$$

where $\Theta_* = \frac{1}{k-1}\Theta_0 + \Theta$, $\nu = \nu_0 + k$, and C_0 define conjugate prior π on m, M, C

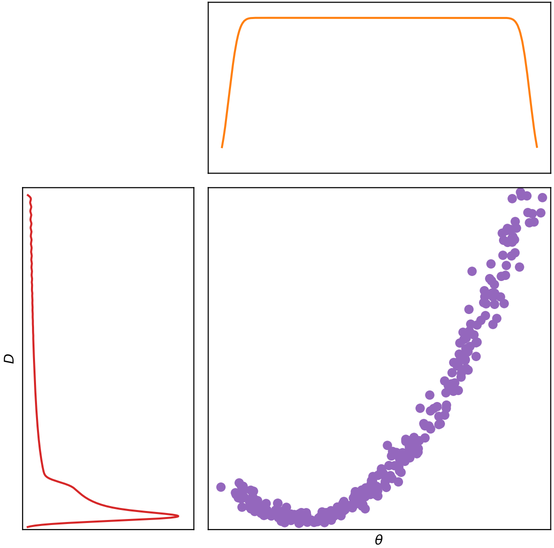


Sequential LSBI

- As we shall see, for non-linear problems, a linear approximation is unlikely to be a good one.
- Sequential methods iteratively improve by focussing effort around observed data D_{obs}.
  - This is orthogonal to amortised approaches
  - More appropriate to cosmology, where there is only one dataset
  - Less appropriate to particle physics/GW
- We are free to choose where to place simulation parameters $\{\theta_i\}$, so it makes sense to choose these so that they generate simulations close to the observed data
- Our current approximation to the posterior is a natural choice.

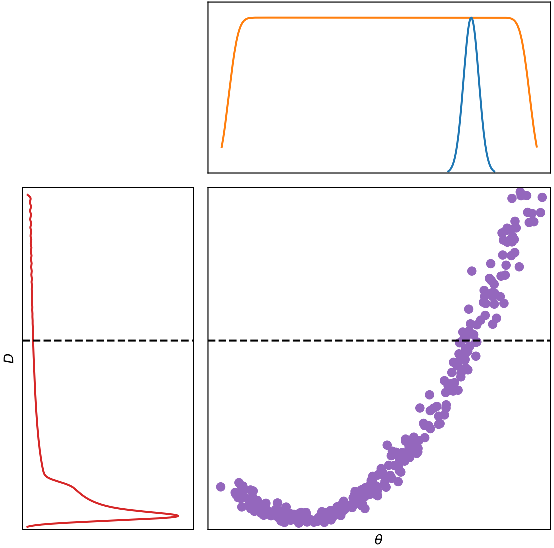
Example of this on our toy model

- Same model as before



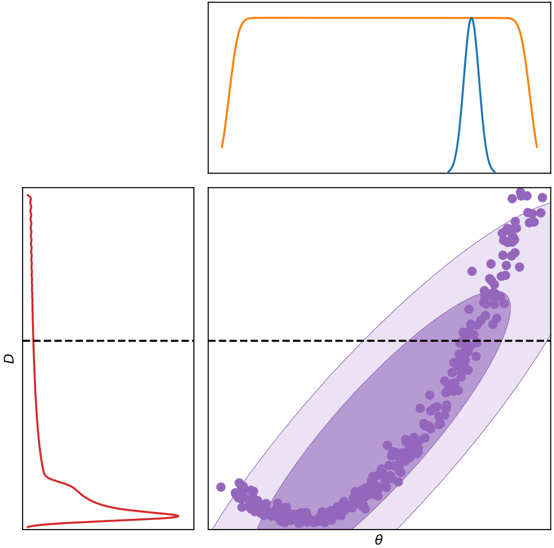
Example of this on our toy model

- Same model as before
- Mark the observed data D_{obs}



Example of this on our toy model

- Same model as before
- Mark the observed data D_{obs}
- Fit a model using `lsbi`



Example of this on our toy model

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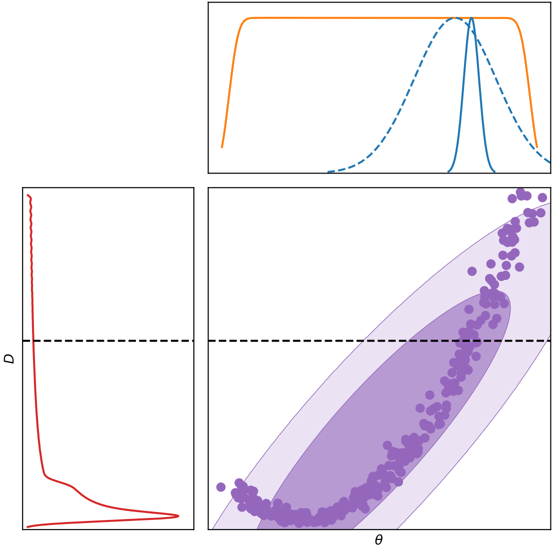
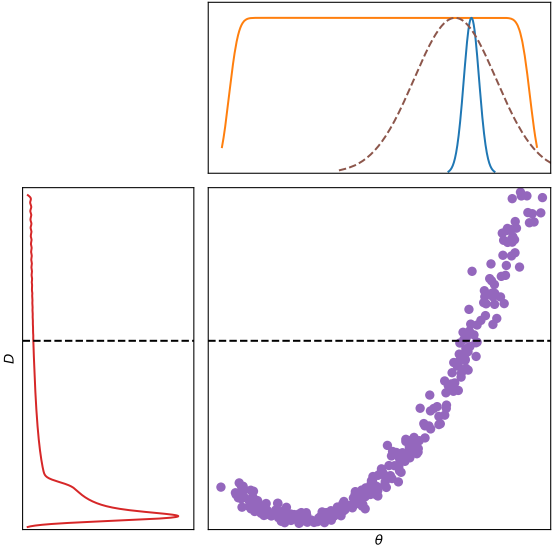
- Mark the observed data D_{obs}
- Fit a model using `lsbi`
- Evaluate the posterior (cheap as linear)



Example of this on our toy model

- Same model as before
- Mark the observed data D_{obs}
- Fit a model using `lsbi`
- Evaluate the posterior (cheap as linear)
- Now use this posterior to pick $\{\theta_i\}$
- Generate $\{D_i\}$ from original simulator



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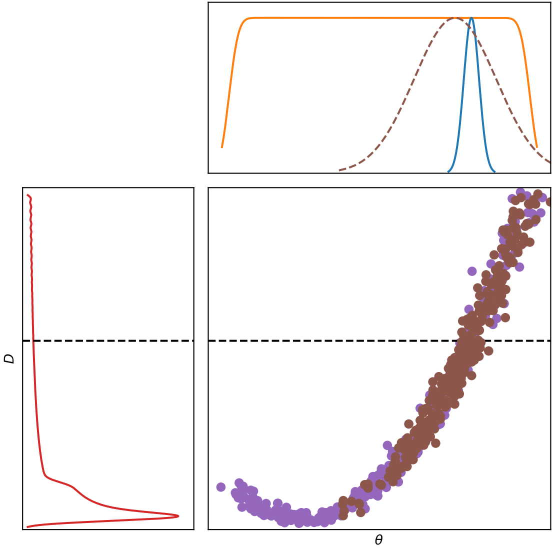
- Fit `lsbi` to these



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- Fit a model using `lsbi`
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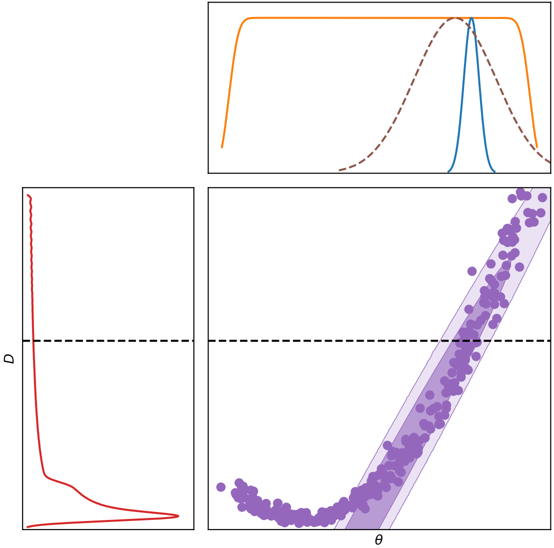
- Fit `lsbi` to these
- Evaluate the new posterior



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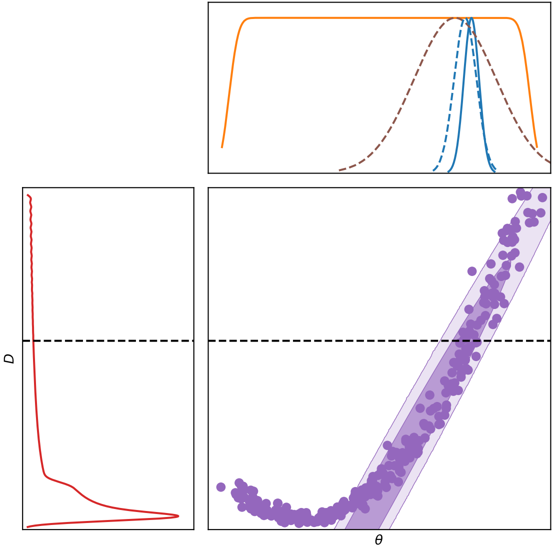
- Iterate



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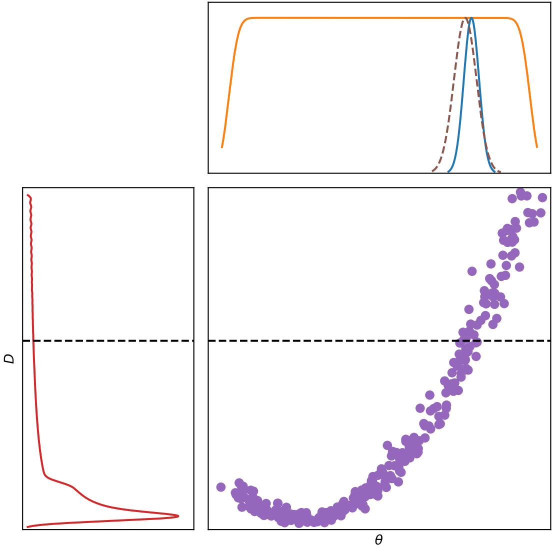

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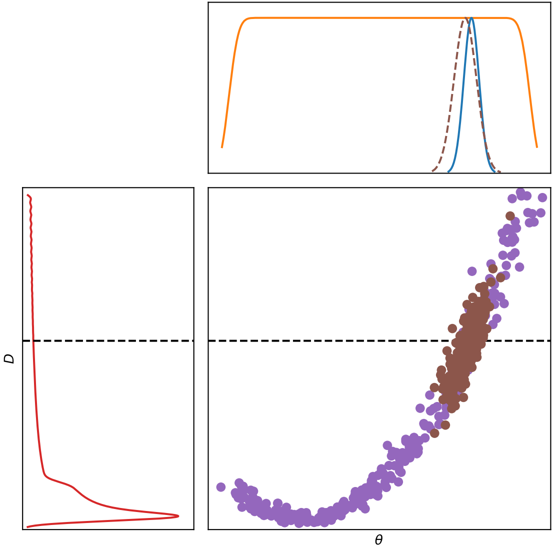

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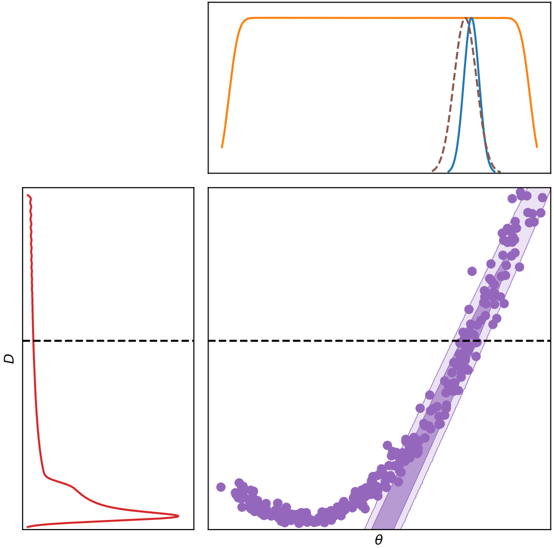

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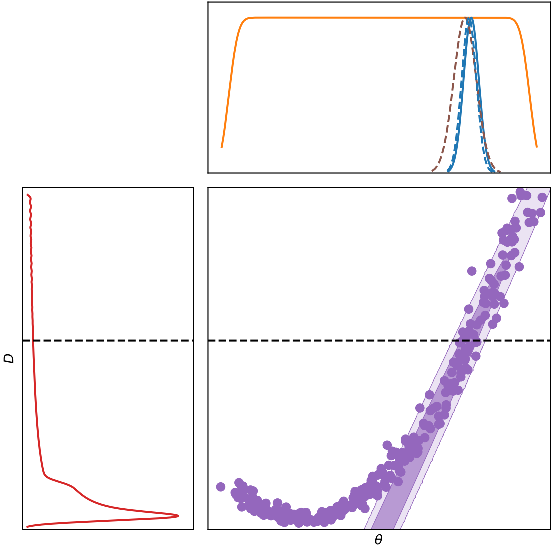

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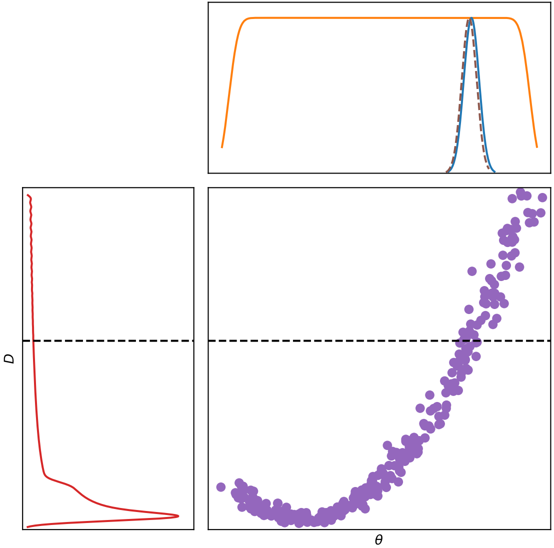

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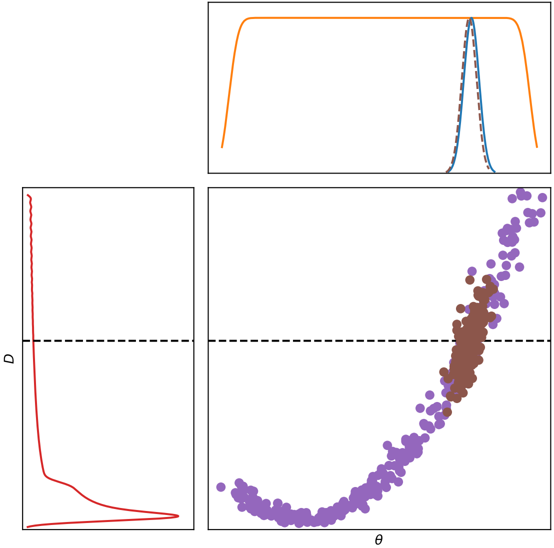

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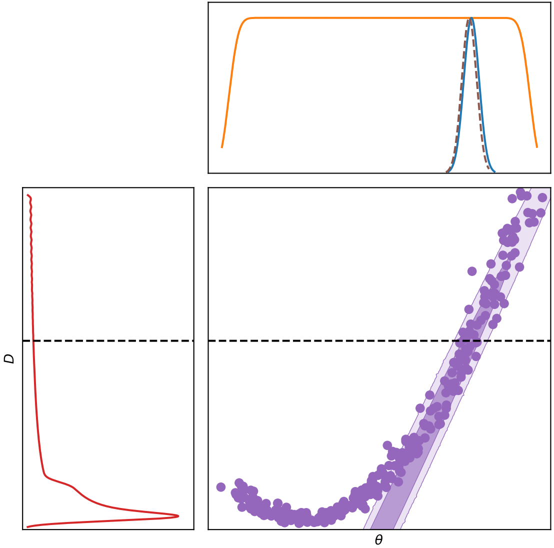

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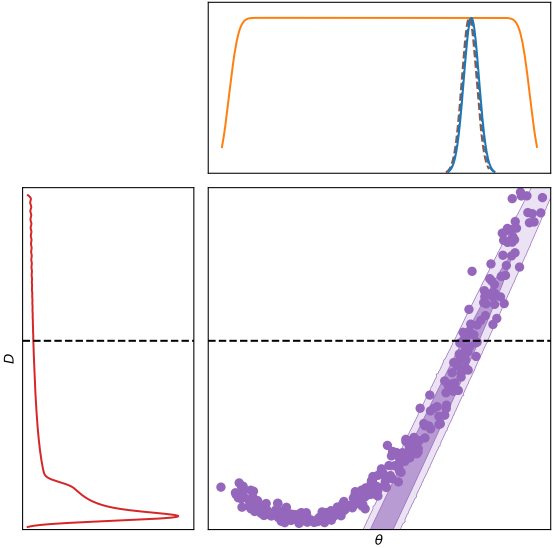
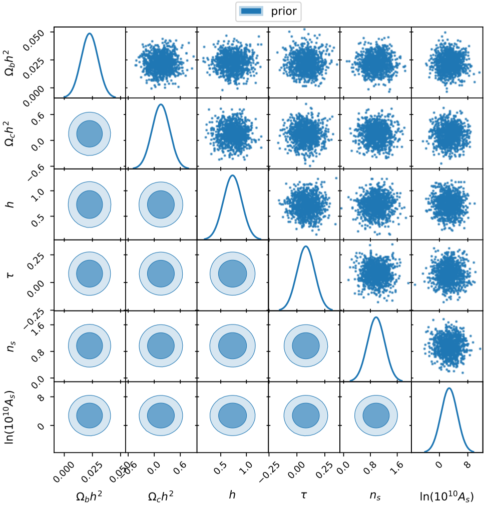


Example of this on the CMB

- Now apply this to a "real" cosmology example, inferring ΛCDM from the CMB
- Unfortunately generative planck likelihoods do not exist yet
- Consider a cosmic-variance limited, temperature-only, full sky CMB experiment with no foregrounds
- This is a $n = 6$, $d = 2500$ non-linear problem
  - No compression needed
- Apply the above procedure
- Slight bias these results, but this can be fixed by marginalising over m, M, C, rather than taking point estimates.



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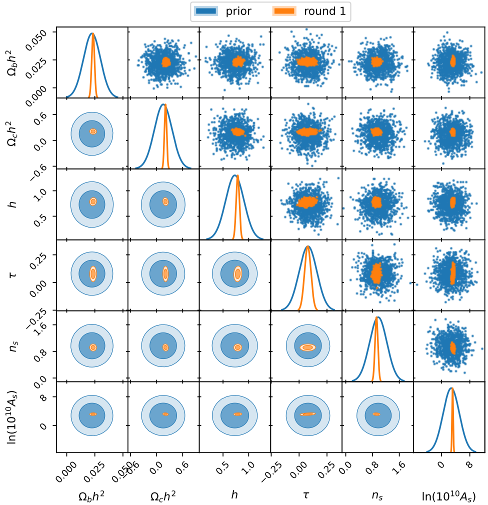

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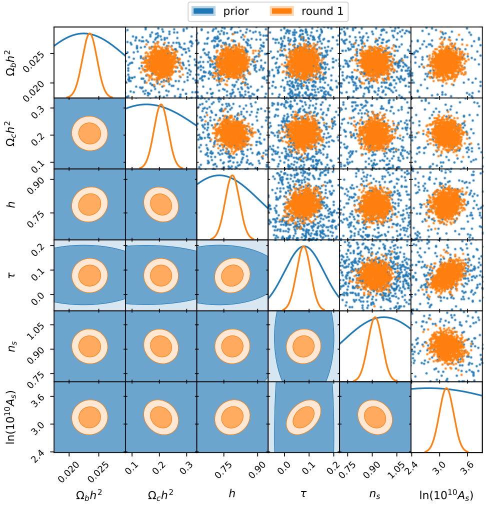

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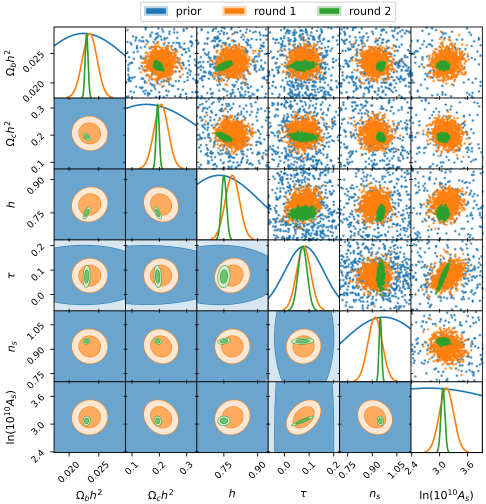

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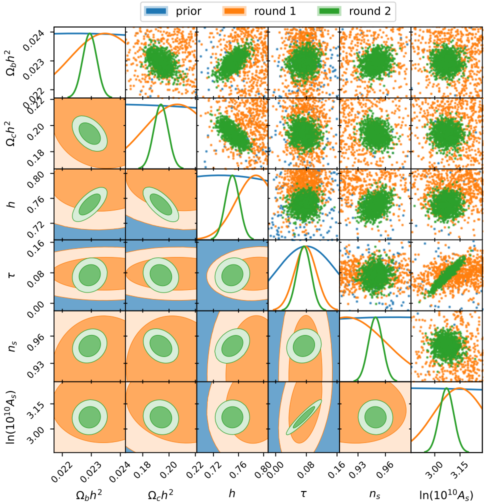

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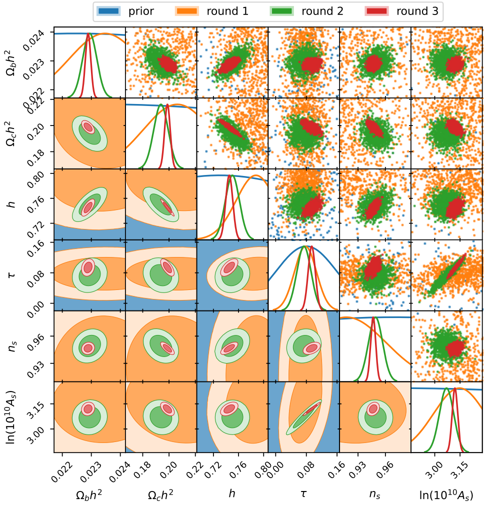

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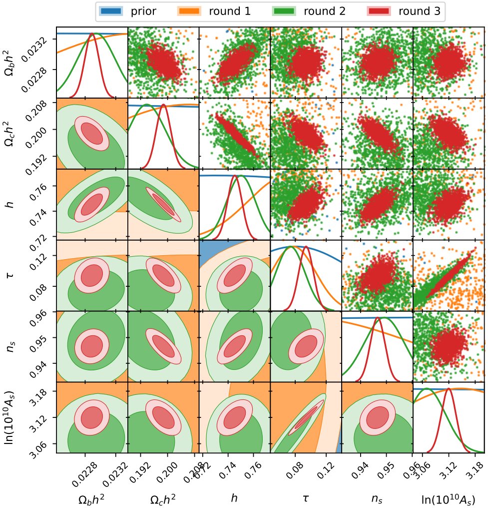

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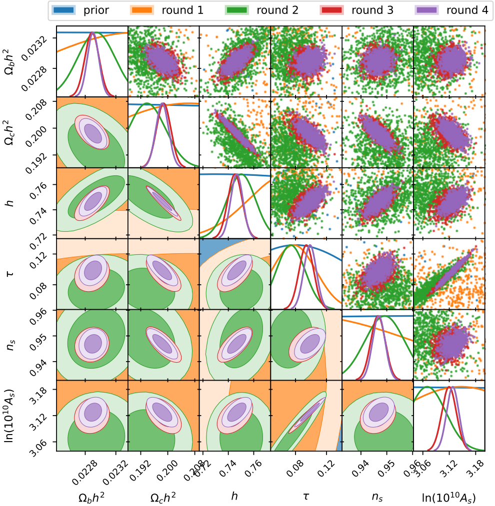

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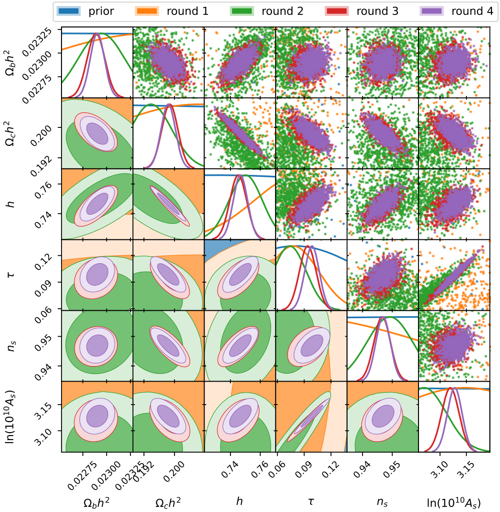

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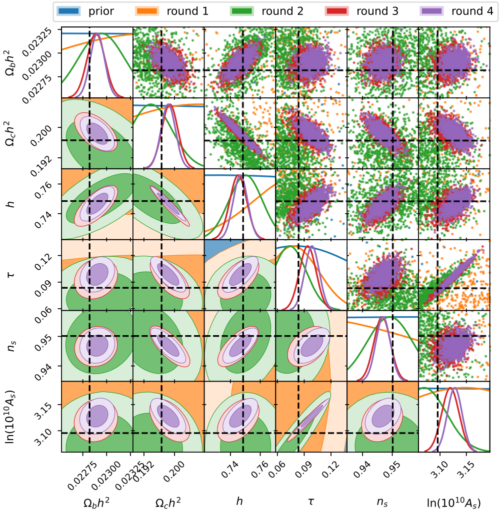

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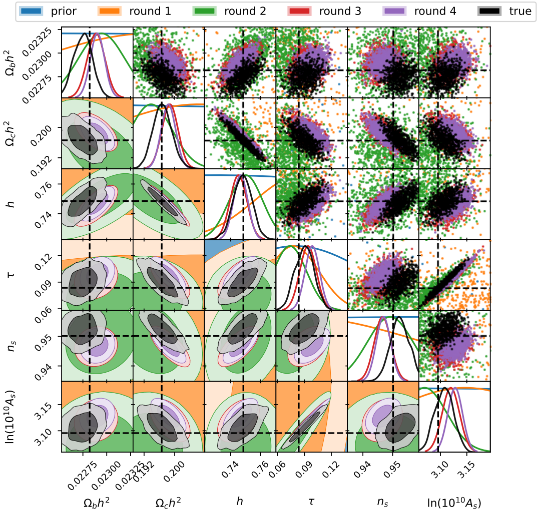

lsbi: linear simulation based inference

Code details

- lsbi is a pip-installable python package
- it extends scipy.stats.multivariate_normal
  - vectorised distributions with (broadcastable) arrays of mean and cov
  - .marginalise(...) and .condition(...) methods
  - Plotting functionality
- Implements LinearModel class with .prior(), .likelihood(theta), .posterior(D) & .evidence() methods which return distributions
- Also implement MixtureModel
- Under active develpoment
  - Open source
  - Continuous integration
- github.com/handley-lab/lsbi

Where next?

- Paper being written up
  - soft deadline for Nicolas' MPhil start in October
  - hard deadline for PhD applications
- Include realistic CMB simulation effects (foregrounds)
- Extend to more examples (BAO, SNe)
- How does LSBI contribute to the question of compression
- Explore limits of d and n
- Explore mixture modelling for real nonlinear effects
- If the posterior is the answer, what is the question?
- Importance sampling?
- Model comparison?

Conclusions

github.com/handley-lab

- **Introduction to `lsbi`:** A linear simulation-based inference method developed over 18 months by the speaker and collaborators.
- **Benefits of Linear SBI:** Pedagogical value, practical examples with known ground truths, competitive accuracy, speed, and interpretability compared to neural networks.
- **Mathematical Setup:** Uses a linear generative model to fit simulation data and iteratively refine posterior estimations, demonstrated through toy and cosmology examples.
- `lsbi` **Python Package:** Extends `scipy.stats.multivariate_normal` with functionalities for marginalization, conditioning, and plotting; under active development and open source.
- **Future Directions:** Include realistic CMB simulations, extend to other examples (BAO, SNe), explore parameter limits, mixture modeling, and integrate importance sampling and model comparison.