

Scalable Bayesian Inference

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Outline

Motivation & background

Big n

High-dimensional data (big p)

Typical approaches to big data



- ✿ There is an increasingly immense literature focused on big data

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- * Huge focus on specific settings - e.g., linear regression, labeling images, etc
- * **Bandwagons: most people work on very similar problems, while critical open problems remain untouched**

My focus - probability models

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General probabilistic inference
algorithms for complex data

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- We would like to handle arbitrarily complex probability models

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- Accurate uncertainty quantification (UQ) is a critical issue
- Robustness of inferences also crucial



Bayes approaches

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- ✿ Choosing a prior $\pi(\theta)$ & likelihood $L(Y^{(n)}|\theta)$, the posterior is

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- ✿ Hence, in interesting models the posterior is not available analytically - what to do??

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- Related class of approximations use a Laplace approximation to $\int \pi(\theta) L(Y^{(n)} | \theta) d\theta$

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- Basis of variational Bayes, expectation-propagation & related methods

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- No theory on accuracy of UQ

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- MCMC bypasses need to approximate the marginal likelihood $L(Y^{(n)})$
- Often samples more useful than an analytic form for $\pi_n(\theta)$ anyway
- Can use samples to calculate a wide variety of posterior & predictive summaries of interest

MCMC

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 1. $\theta^* \sim g(\theta^{(t-1)})$ = sample a proposal ($\theta^{(t)}$ =sample at step t)
 2. Accept proposal by letting $\theta^{(t)} = \theta^*$ with probability

$$\min \left\{ 1, \frac{\pi(\theta^*) L(Y^{(n)}|\theta^*)}{\pi(\theta^{(t-1)}) L(Y^{(n)}|\theta^{(t-1)})} \frac{g(\theta^{(t-1)})}{g(\theta^*)} \right\}$$

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- Random walk: $g(\theta^{(t-1)})$ is a distribution centered on $\theta^{(t-1)}$ with a tunable covariance
- HMC/Langevin: Exploit gradient information to generate samples far from $\theta^{(t-1)}$ having high posterior density

MCMC & Computational bottlenecks



- ✿ Time per iteration increases with # of parameters/unknowns

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- Due to the cost of sampling proposal & calculating acceptance probability
- Similar costs occur in most optimization algorithms!
- For example, the computational bottleneck may be attributable to gradient evaluations

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- A well designed MCMC algorithm with a good proposal should ideally exhibit rapid convergence & mixing

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- Draws are auto-correlated - as level of correlation increases, information provided by each sample decreases
- “Slowly mixing” Markov chains have highly autocorrelated draws
- A well designed MCMC algorithm with a good proposal should ideally exhibit rapid convergence & mixing
- Otherwise the Monte Carlo (MC) error in posterior summaries may be high

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- ✿ Also MCMC is an inherently serial algorithm, so naive implementation may require storing & processing all data on one machine
- ✿ Limits ease at which divide-and-conquer strategies can be applied.
- ✿ For the above reasons, it is common to simply state that MCMC is not scalable

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- I'm going to highlight some relevant relevant work starting by focusing on big n problems & then transitioning to big p

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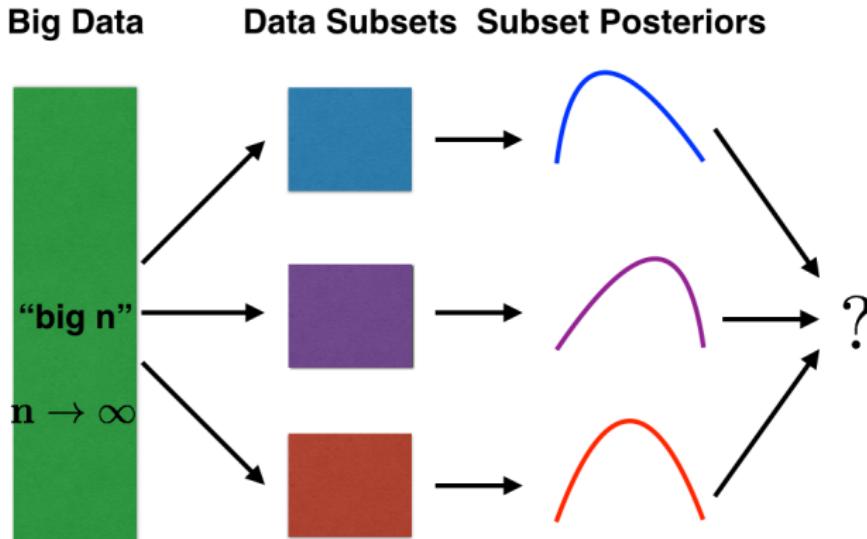
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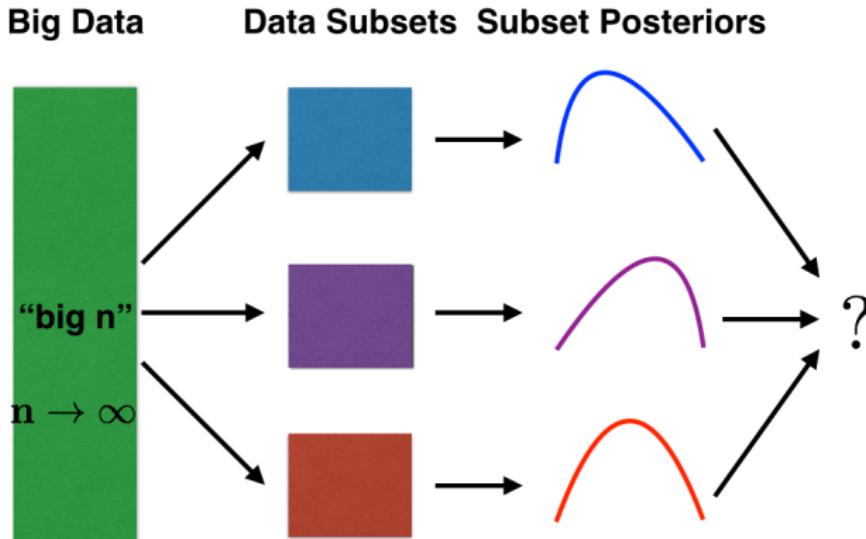
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- **Hybrid algorithms:** run MCMC for a subset of the parameters & use a fast estimate for the others.

Embarrassingly parallel MCMC



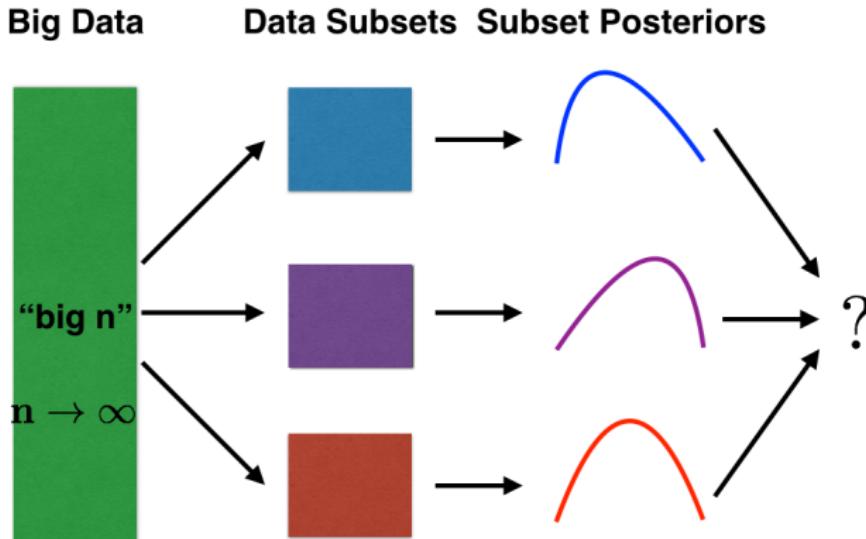
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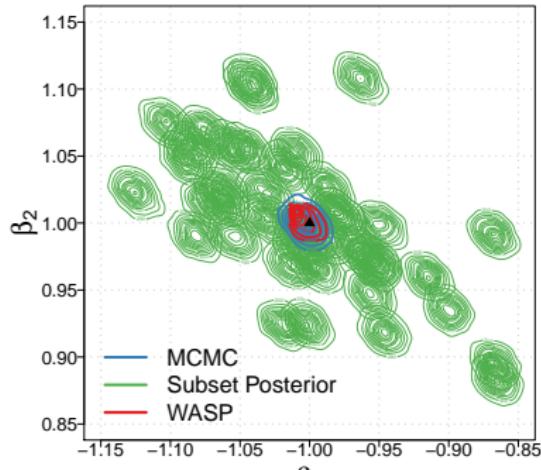
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- ➌ 'Magically' combine the results quickly & simply

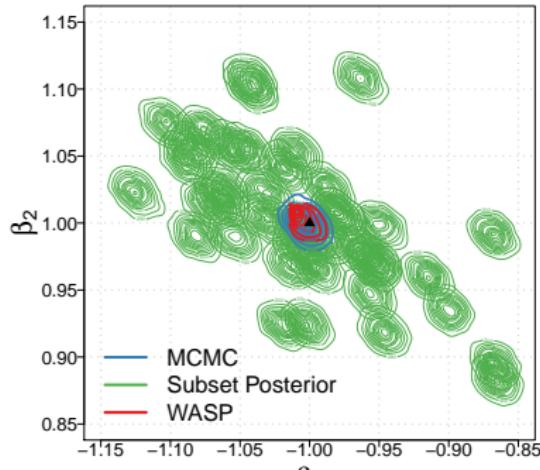
Toy Example: Logistic Regression



$$\text{pr}(y_i = 1 | x_{i1}, \dots, x_{ip}, \theta) = \frac{\exp\left(\sum_{j=1}^p x_{ij} \beta_j\right)}{1 + \exp\left(\sum_{j=1}^p x_{ij} \beta_j\right)}.$$

- Subset posteriors: ‘noisy’ approximations of full data posterior.

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- Subset posteriors: ‘noisy’ approximations of full data posterior.
- ‘Averaging’ of subset posteriors reduces this ‘noise’ & leads to an accurate posterior approximation.

Stochastic Approximation

- Full data posterior density of *inid* data $Y^{(n)}$

$$\pi_n(\theta \mid Y^{(n)}) = \frac{\prod_{i=1}^n p_i(y_i \mid \theta) \pi(\theta)}{\int_{\Theta} \prod_{i=1}^n p_i(y_i \mid \theta) \pi(\theta) d\theta}.$$

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$$Y^{(n)} = (Y_{[1]}, \dots, Y_{[j]}, \dots, Y_{[k]}).$$

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- ✿ Subset posterior density for j th data subset

$$\pi_m^r(\theta \mid Y_{[j]}) = \frac{\prod_{i \in [j]} (p_i(y_i \mid \theta))^r \pi(\theta)}{\int_{\Theta} \prod_{i \in [j]} (p_i(y_i \mid \theta))^r \pi(\theta) d\theta}.$$

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- Full data posterior density of *inid* data $Y^{(n)}$

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- Divide full data $Y^{(n)}$ into k subsets of size m :

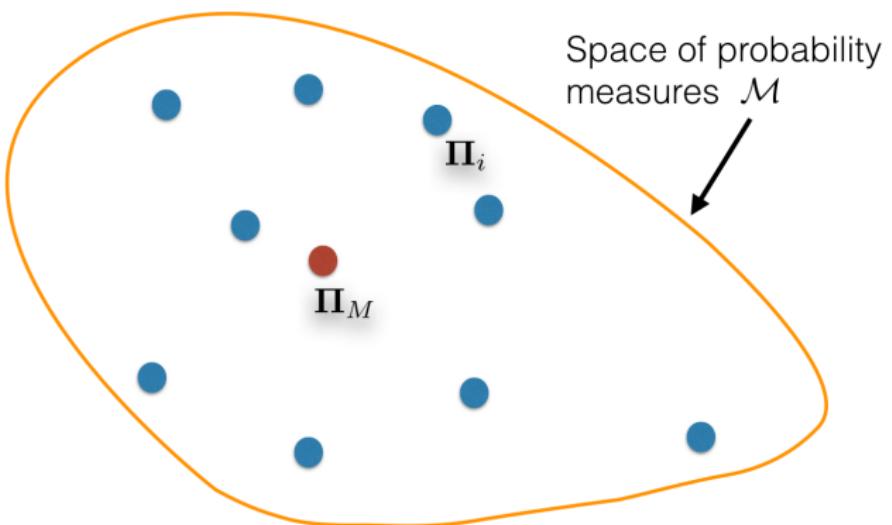
$$Y^{(n)} = (Y_{[1]}, \dots, Y_{[j]}, \dots, Y_{[k]}).$$

- Subset posterior density for j th data subset

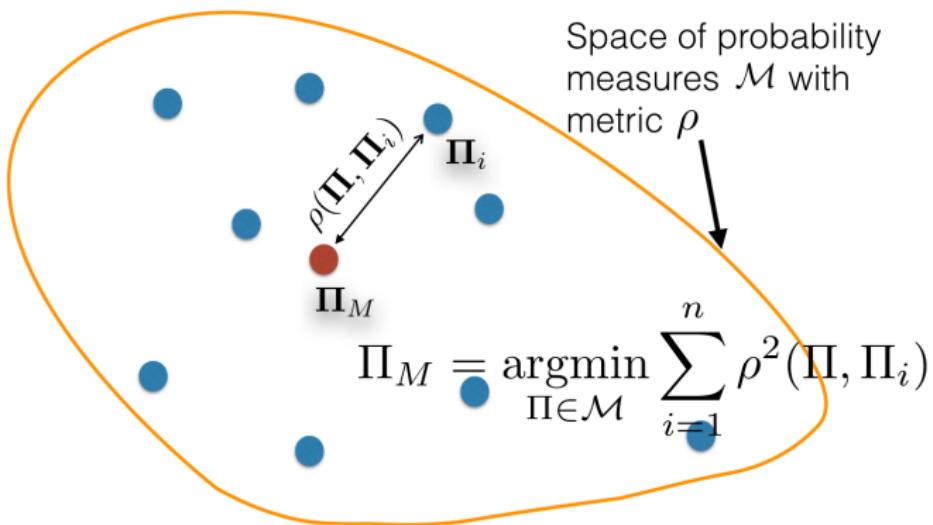
$$\pi_m^{\gamma}(\theta \mid Y_{[j]}) = \frac{\prod_{i \in [j]} (p_i(y_i \mid \theta))^{\gamma} \pi(\theta)}{\int_{\Theta} \prod_{i \in [j]} (p_i(y_i \mid \theta))^{\gamma} \pi(\theta) d\theta}.$$

- $\gamma = O(k)$ - chosen to minimize approximation error

Barycenter in Metric Spaces



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Wasserstein barycenter of Subset Posteriors (WASP)



Srivastava, Li & Dunson (2015)

• 2-Wasserstein distance between $\mu, \nu \in \mathcal{P}_2(\Theta)$

$$W_2(\mu, \nu) = \inf \left\{ \left(\mathbb{E}[d^2(X, Y)] \right)^{\frac{1}{2}} : \text{law}(X) = \mu, \text{law}(Y) = \nu \right\}.$$

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$$\bar{\Pi}_n^\gamma(\cdot | Y^{(n)}) = \operatorname*{argmin}_{\Pi \in \mathcal{P}_2(\Theta)} \frac{1}{k} \sum_{j=1}^k W_2^2(\Pi, \Pi_m^\gamma(\cdot | Y_{[j]})). \quad [\text{Aguech \& Carlier (2011)}]$$

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- Plugging in $\hat{\Pi}_m^\gamma(\cdot | Y_{[j]})$ for $j = 1, \dots, k$, a linear program (LP) can be used for fast estimation of an atomic approximation!

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- We can avoid such smoothing & use sparse LP solvers - negligible computation cost compared to sampling

WASP: Theorems

Theorem (Subset Posteriors)

Under “usual” regularity conditions, there exists a constant C_1 independent of subset posteriors, such that for large m ,

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- Conditions: standard, mild conditions on likelihood + prior finite 2nd moment & uniform integrability of subset posteriors

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- ✿ Not clear what happens when we start substituting in approximations - may diverge etc

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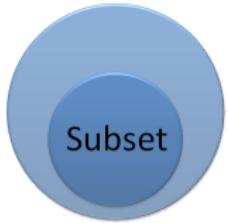
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Ex 1: Approximations using subsets

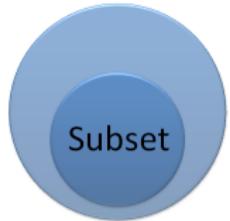


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for randomly chosen subset $V \subset \{1, \dots, n\}$.

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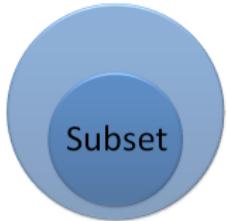
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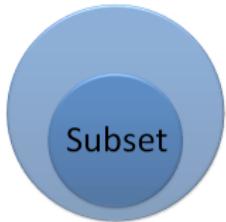
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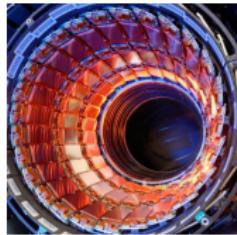


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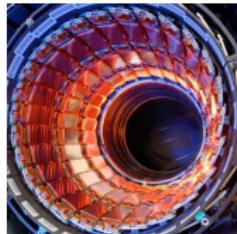
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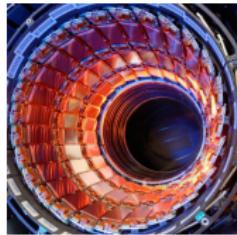
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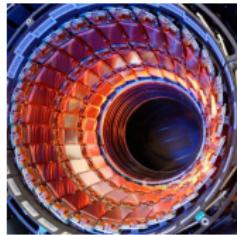
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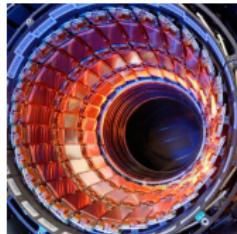
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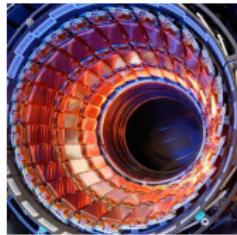
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- As budget increases & loss focused more on tails (e.g., for interval estimation), optimal $|V|$ increases

Application 2: Mixture models & tensor factorizations

A hand-drawn diagram showing a 3D cube labeled "TENSOR" on its base. To its right is the equation $= \text{PARAFAC} + \text{PARAFAC}$, where each "PARAFAC" term is represented by a smaller 3D cube.

- We also considered a nonparametric Bayes model:

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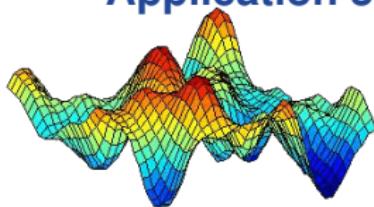
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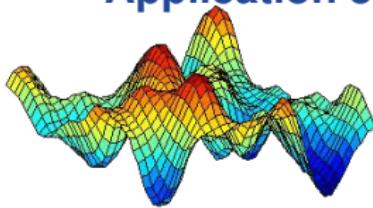
- Dunson & Xing (2009) - a data augmentation Gibbs sampler
- Sampling latent classes computationally prohibitive for huge n
- Use adaptive Gaussian approximation - avoid sampling individual latent classes
- We have shown Assumptions 1-2, Assumption 2 result more general than this setting
- Improved computation performance for large n**

Application 3: Low rank approximation to GP



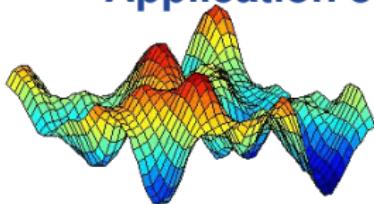
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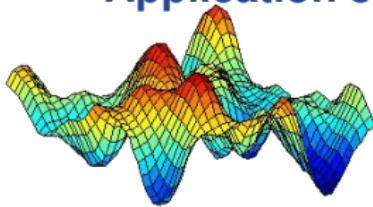
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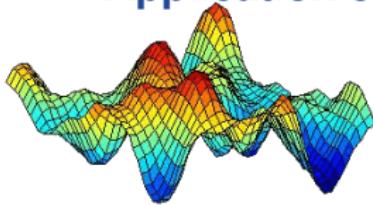
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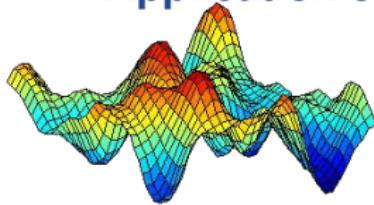
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- Less accurate approximations clearly superior in practice for small computational budget

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- Robustness: one topic we haven't discussed yet is robustness

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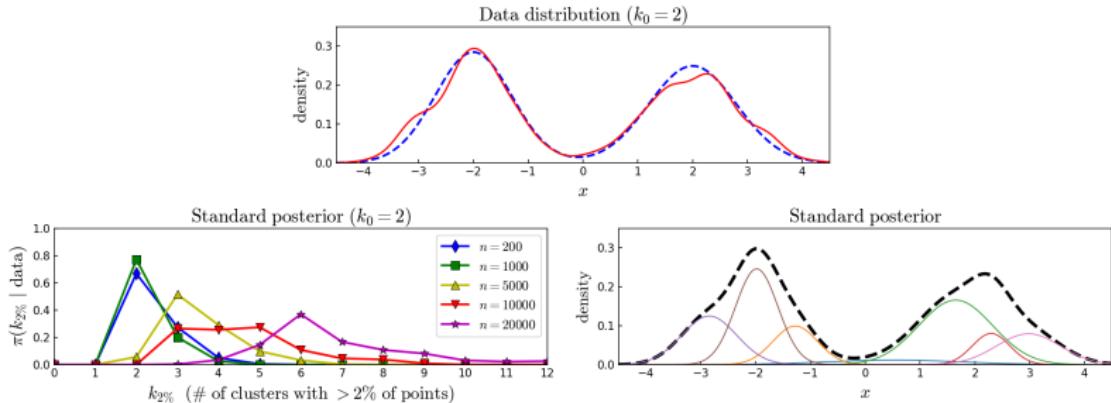
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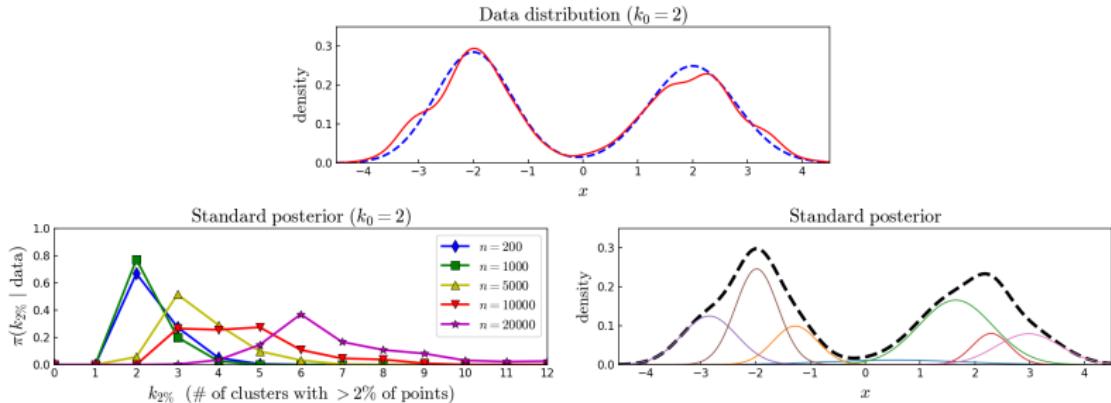
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- **Appealing to tweak Bayesian paradigm to be inherently more robust**

Example: Perturbed mixture of Gaussians



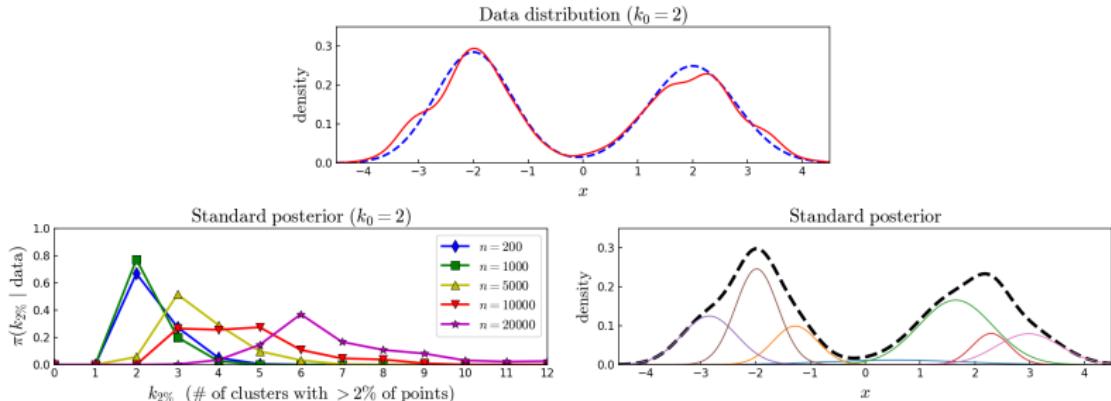
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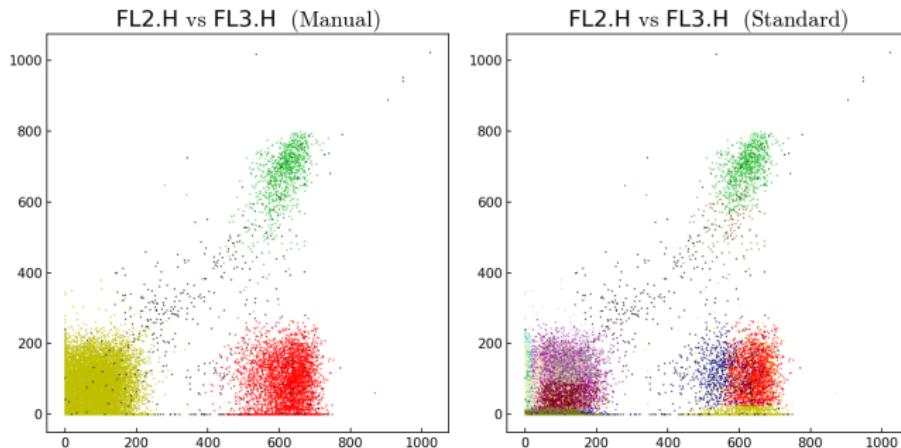
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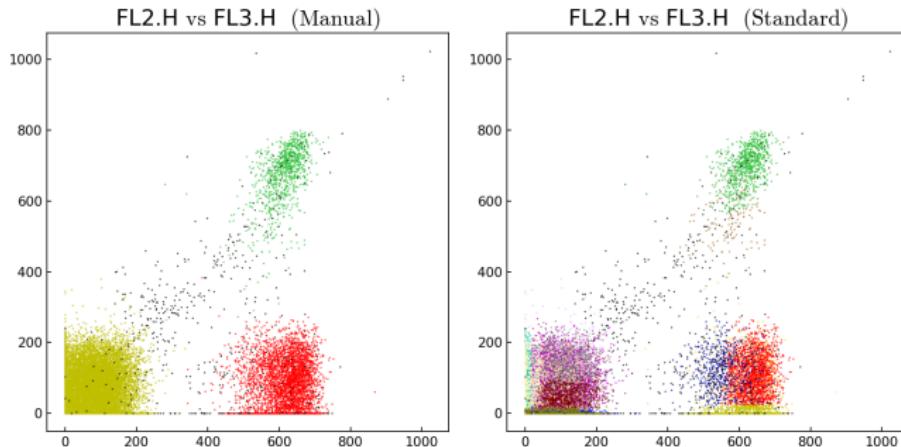
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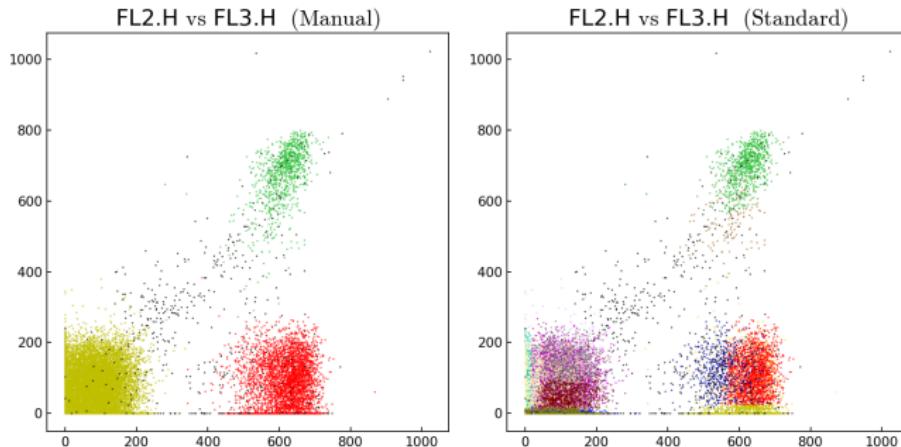
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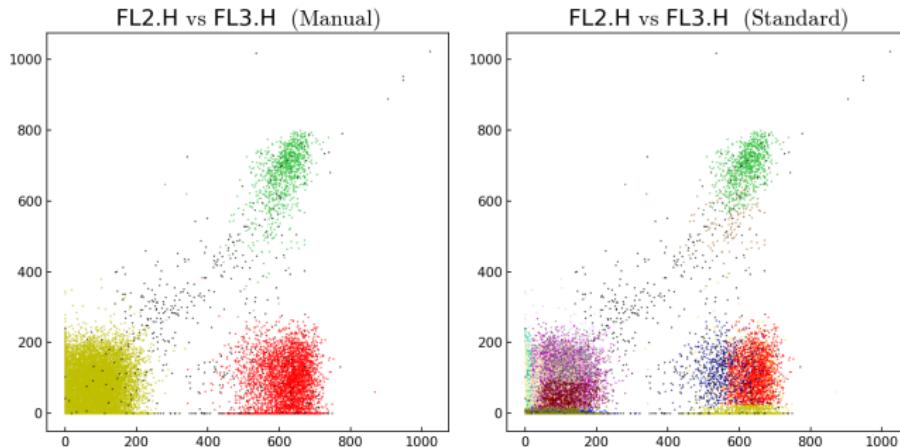
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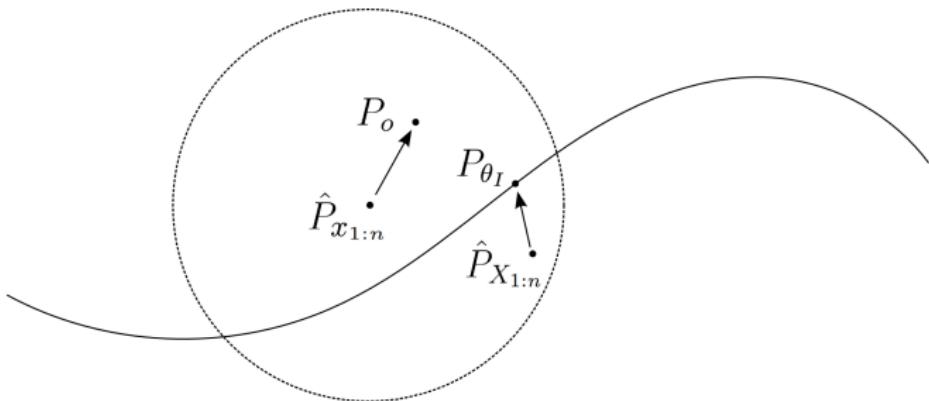
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 - ~ Many models are idealizations that are known to be inexact, but have interpretable parameters that provide insight into the questions of interest.

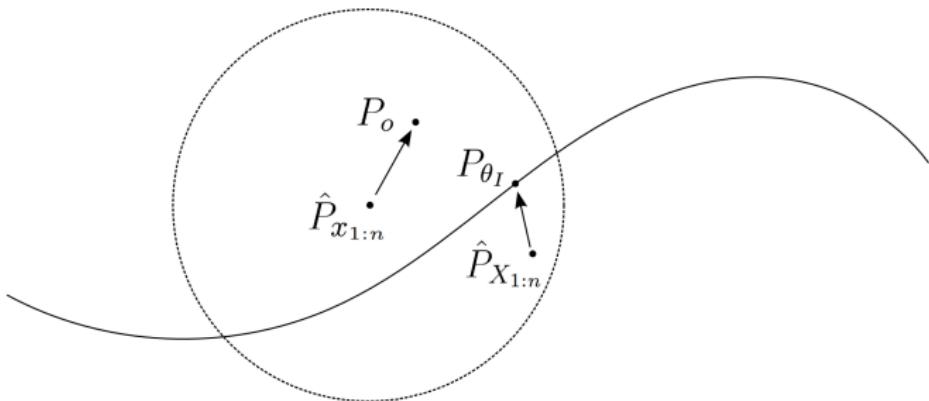
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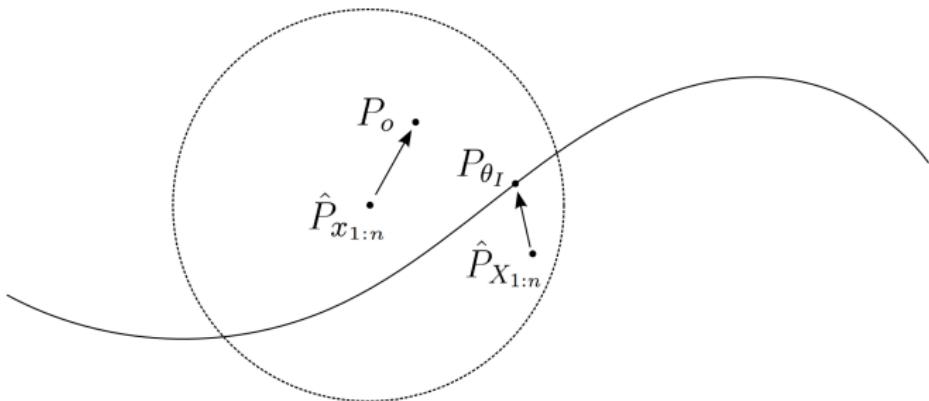
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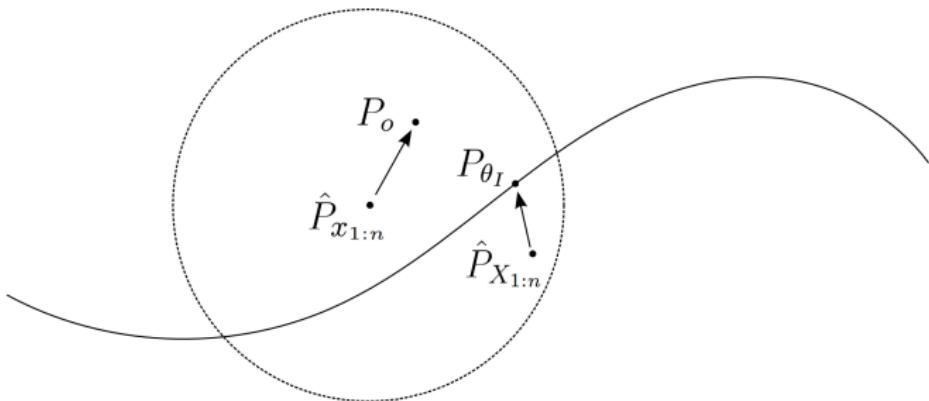
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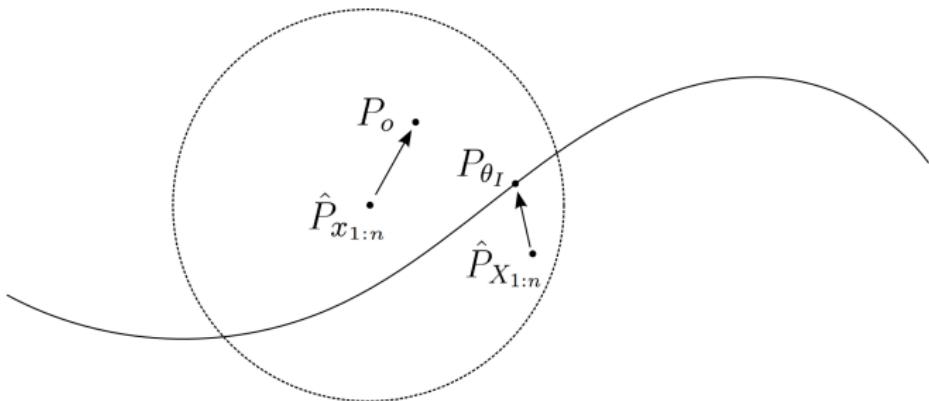
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- Suppose X_1, \dots, X_n i.i.d. $\sim P_{\theta_I}$ are unobserved *idealized data*.
- However, the *observed data* x_1, \dots, x_n are actually a slightly corrupted version of X_1, \dots, X_n in the sense that
Big n $d(\hat{P}_{X_{1:n}}, \hat{P}_{x_{1:n}}) < R$ for some statistical distance $d(\cdot, \cdot)$.

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- More generally, consider

$$\pi(\theta | d_n(X_{1:n}, x_{1:n}) < R)$$

where $d_n(X_{1:n}, x_{1:n}) \geq 0$ is some measure of the discrepancy between $X_{1:n}$ and $x_{1:n}$.

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 - ~ MCMC is also straightforward

Toy example: Bernoulli trials

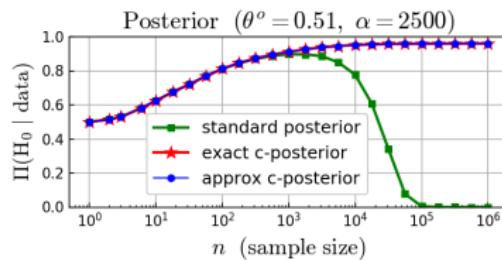
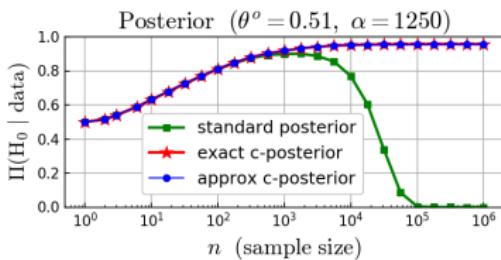
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- But x_1, \dots, x_n are corrupted and behave like $\text{Bernoulli}(0.51)$ samples.
- The c-posterior is robust to this, but the standard posterior is not.



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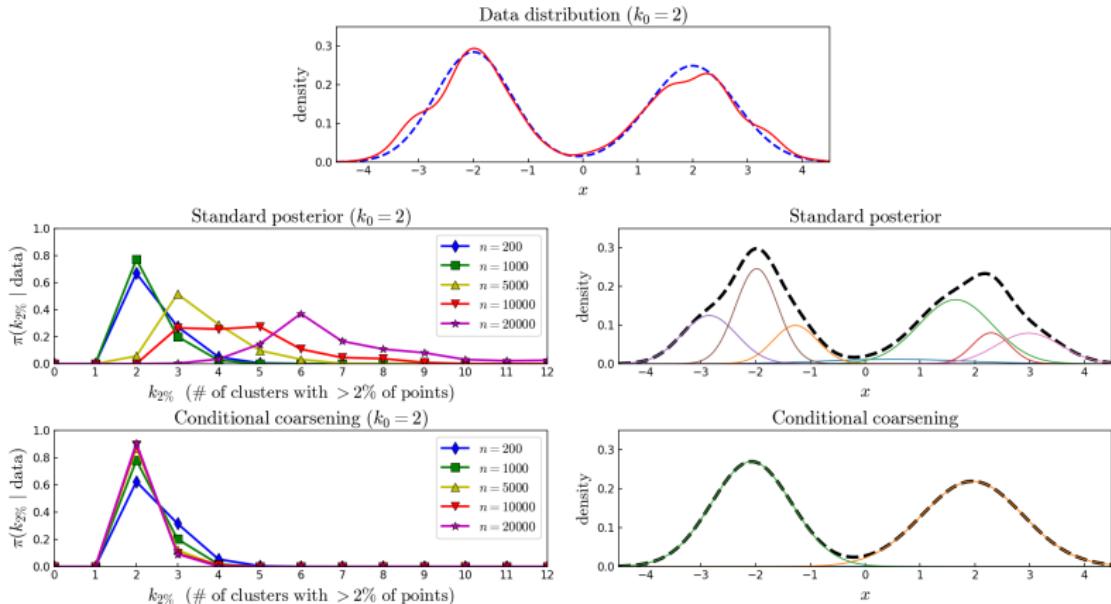
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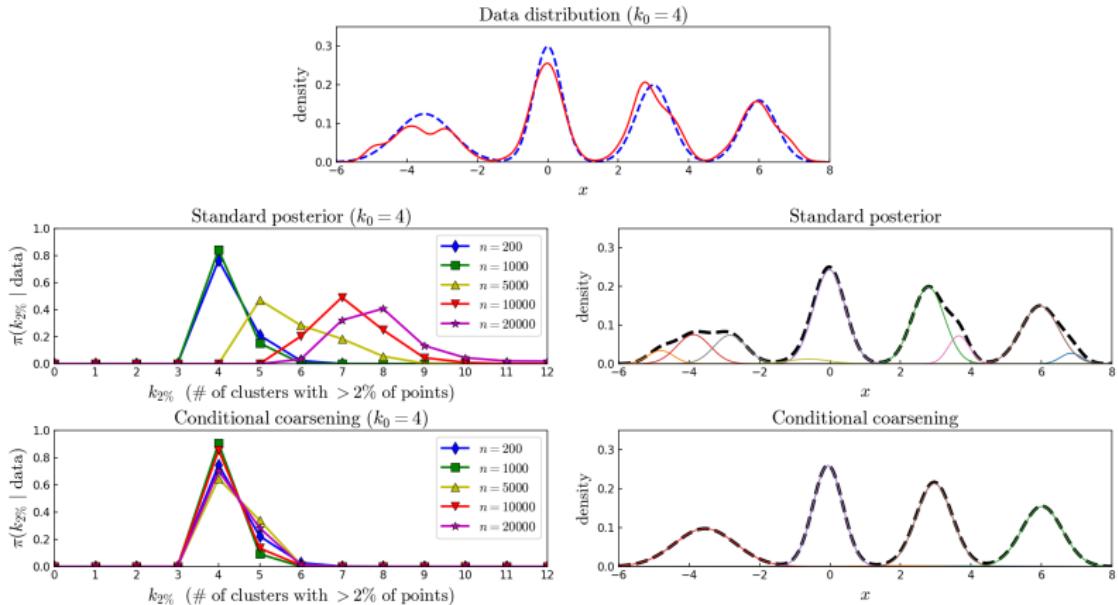
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- * A straightforward MCMC algorithm can be used for computation
- * Scales well to large datasets
- * EP-MCMC, a-MCMC etc can be used to enhance scalability

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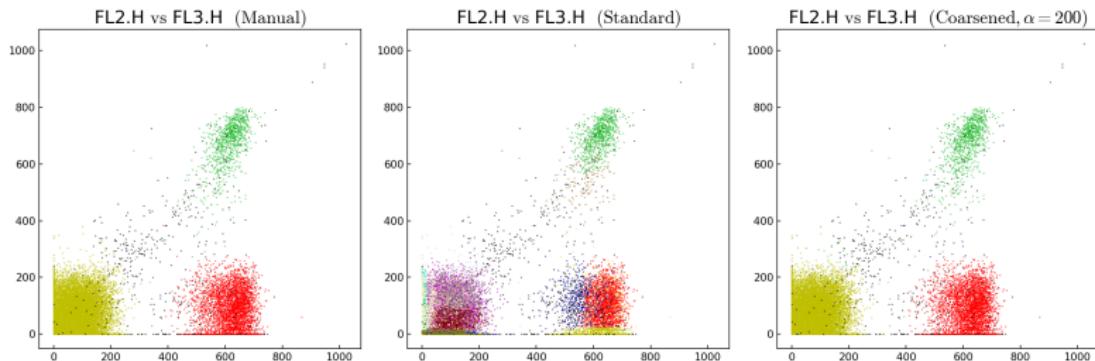


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Results: Flow cytometry clustering

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Table 1: Average F-measures on the flow cytometry test set (GvHD datasets 7–12).

	7	8	9	10	11	12
Standard	0.532	0.478	0.619	0.453	0.542	0.585
Coarsened	0.667	0.875	0.931	0.998	0.989	0.993

- Clustering on test datasets closely matches manual ground truth.
- Use F-measure to quantify similarity of partitions \mathcal{A} and \mathcal{B} :

$$F(\mathcal{A}, \mathcal{B}) = \sum_{A \in \mathcal{A}} \frac{|A|}{N} \max_{B \in \mathcal{B}} \frac{2|A \cap B|}{|A| + |B|}.$$

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- Also provides a motivation for doing Bayesian inferences based on subsamples

Hybrid high-dimensional density estimation



Ye, Canale & Dunson (2016, AISTATS)

- $y_i = (y_{i1}, \dots, y_{ip})^T \sim f$ with p large & f an unknown density

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- Instead use hybrid of Gibbs sampling & fast multiscale SVD
- **Scalable, excellent mixing & empirical/predictive performance**

Outline

Motivation & background

Big n

High-dimensional data (big p)

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- Bayes for big p is a huge topic - I'll just provide some vignettes to give a flavor

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 2. **Penalized estimation/shrinkage**

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- Get a list of discoveries & hopefully run follow-up studies to verify

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Independent Screening - Continued

- Very appealing in its simplicity
- Very widely used
- Many false positives & negatives; for sparse data false negatives huge problem
- Just considering a pair of variables at a time leads to limited insights

Problems with classical approaches

- Consider the canonical linear regression problem:

$$y_i = x_i' \beta + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2),$$

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- For $p > n$ a unique MLE doesn't exist

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- In a Bayesian approach, we choose a prior probability distribution $\pi(\beta)$ characterizing our uncertainty in β prior to observing the current data
- Then, we would use Bayes rule to update the prior with information in the likelihood:

$$\pi(\beta|Y, X) = \frac{\pi(\beta)L(Y|X, \beta)}{\int \pi(\beta)L(Y|X, \beta) d\beta} = \frac{\pi(\beta)L(Y|X, \beta)}{L(Y|X)},$$

where $L(Y|X, \beta)$ is the likelihood & $L(Y|X)$ is the marginal likelihood

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- The posterior mean is $\tilde{\beta} = (\sigma^2 \Sigma_0^{-1} + X'X)^{-1} X'Y$, which is a weighted average of 0 and $\hat{\beta} = (X'X)^{-1} X'Y$.

Penalized estimation

* We can get the same estimator for β by solving:

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- Such estimators introduce some bias while reducing the variance a lot to improve mean square error

L1 - Lasso sparse estimation

- The above penalized loss function can be generalized as

$$\tilde{\beta} = \operatorname{argmin}_{\beta} \|Y - X\beta\|_2^2 + p_{\lambda}(\beta),$$

where $p_{\lambda}(\beta)$ is a *penalty* term - L2 in the case discussed above

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- Parallel Bayesian literature on shrinkage priors - horseshoe, generalized double Pareto, Dirichlet-Laplace, etc

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- Datta & Dunson (2016, *Biometrika*) - develop such approaches for huge dimensional sparse count data arising in genomics

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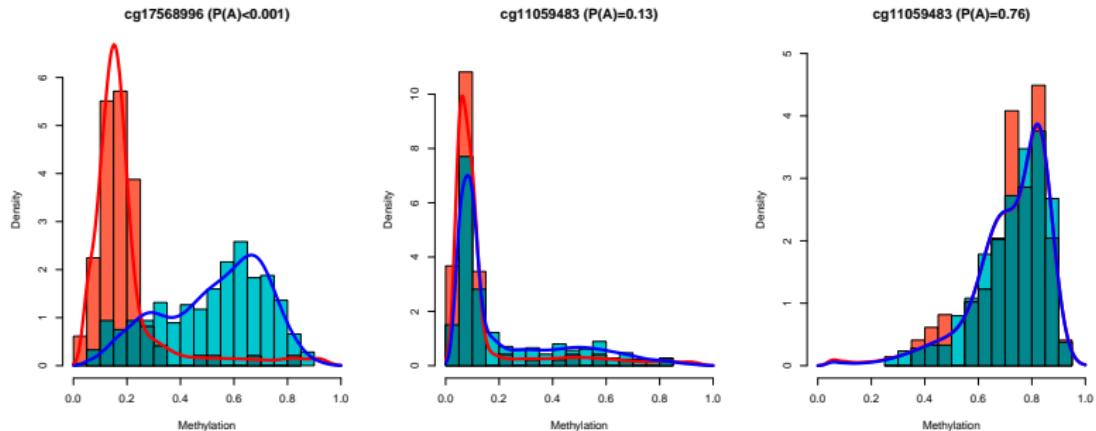
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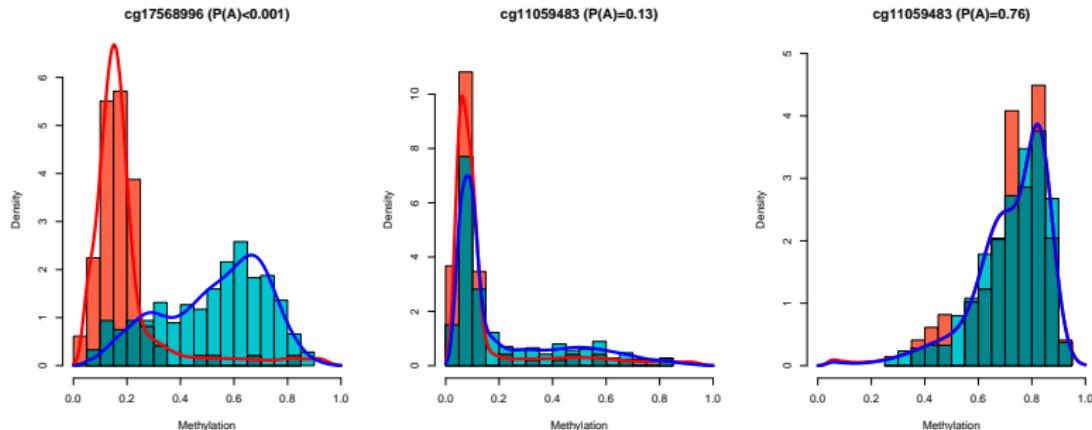
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 3. provide a way to deal with intractable $p \gg n$ problems

Application 1: DNA methylation arrays



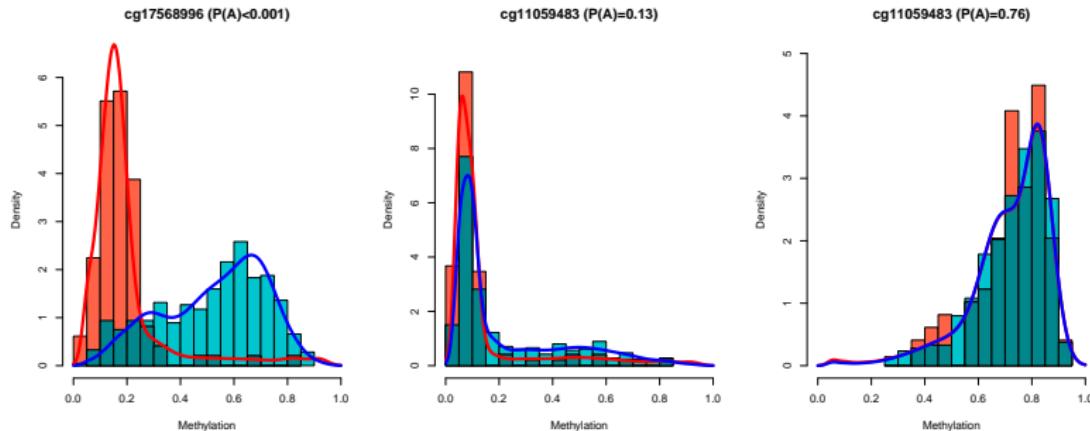
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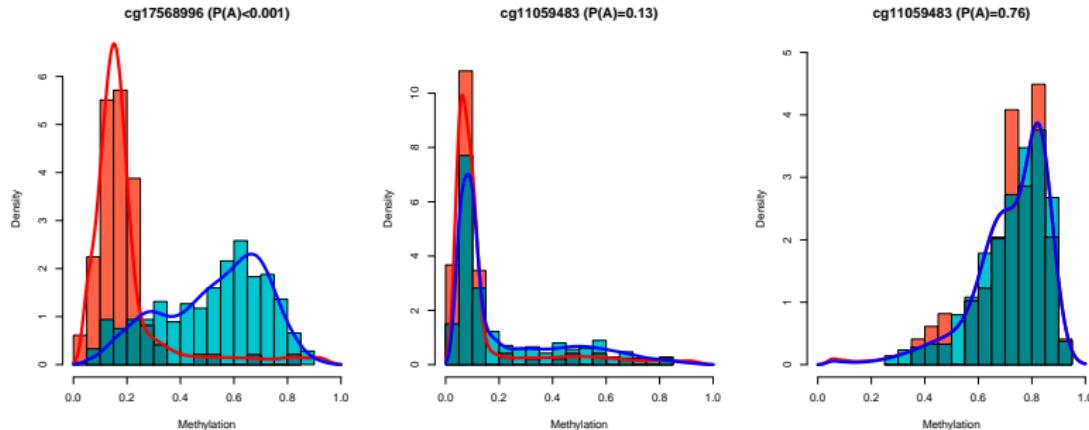
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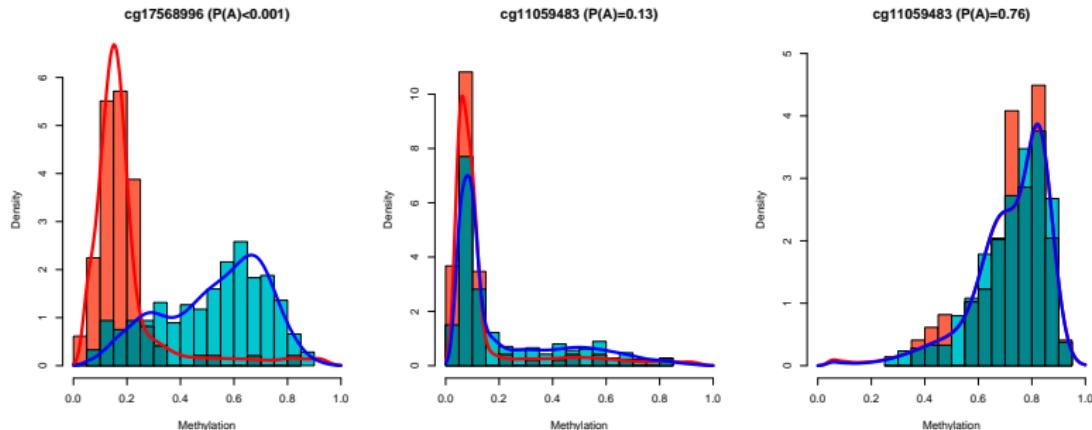
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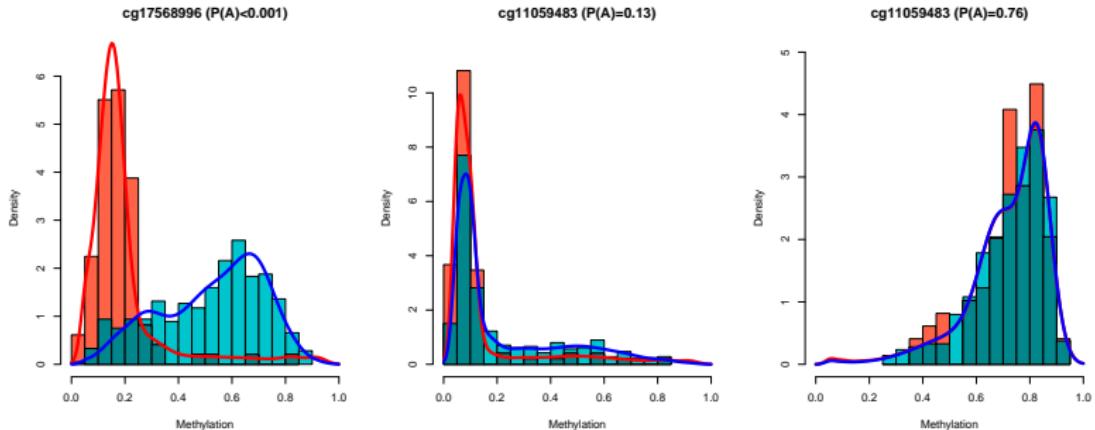
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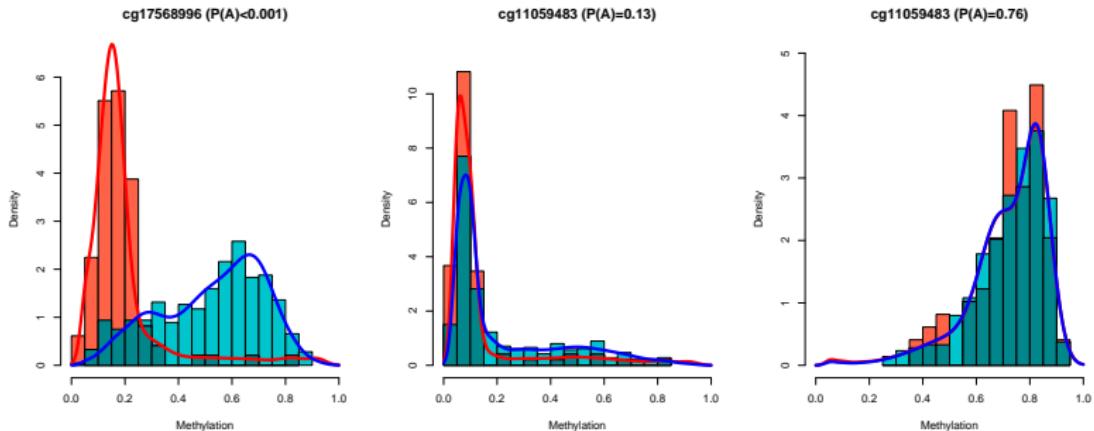
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- Clearly distributions exhibit multimodality & skewness

Comments



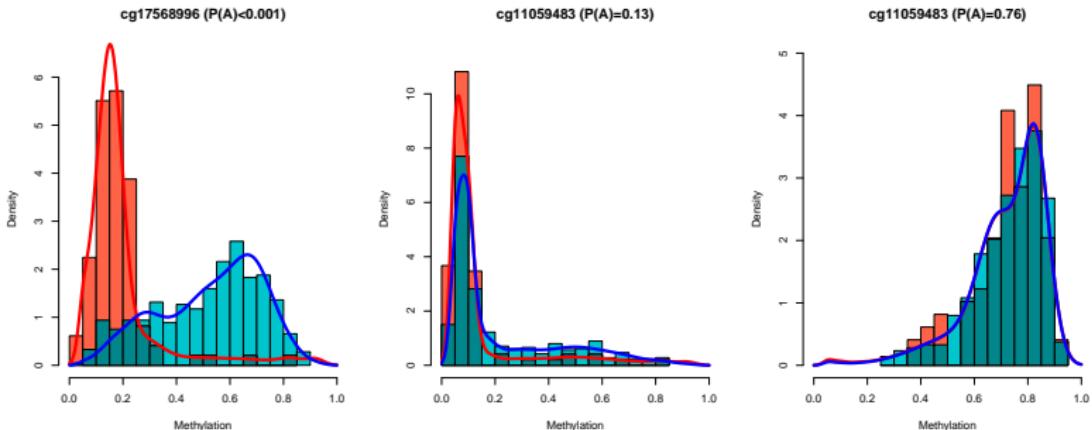
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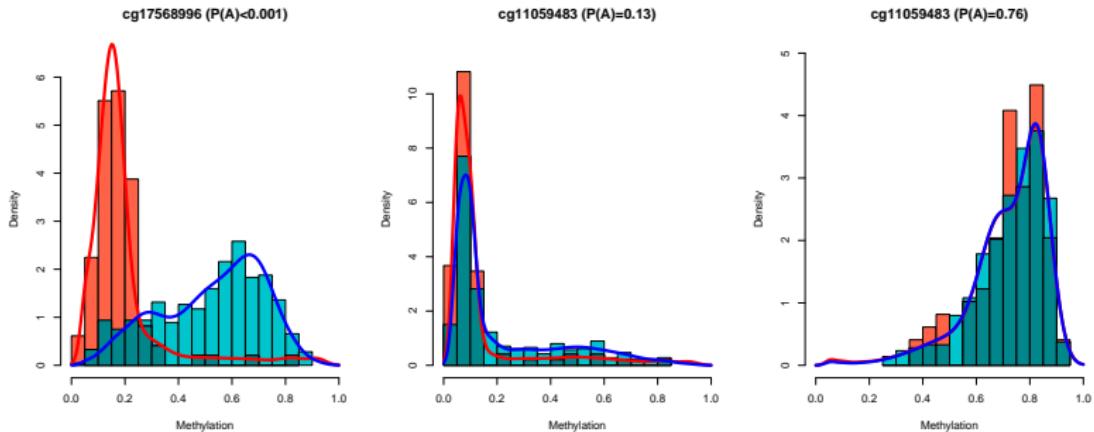
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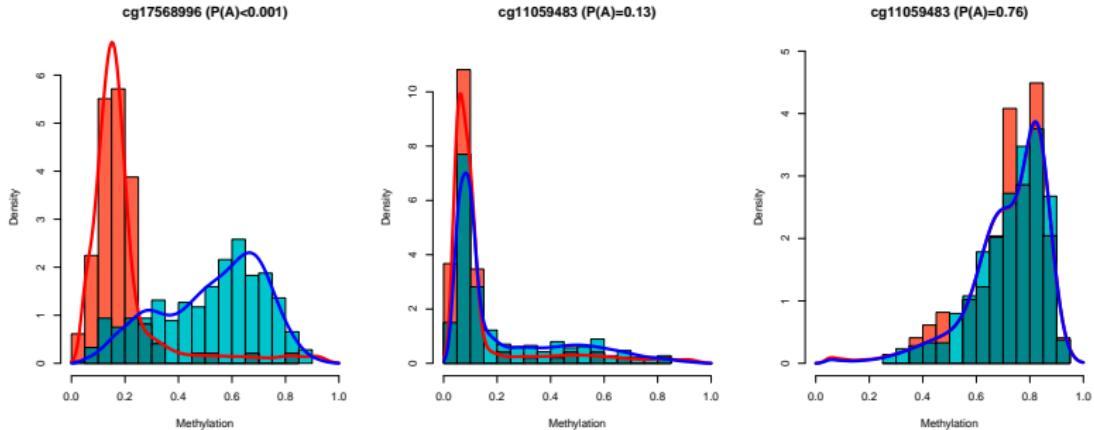
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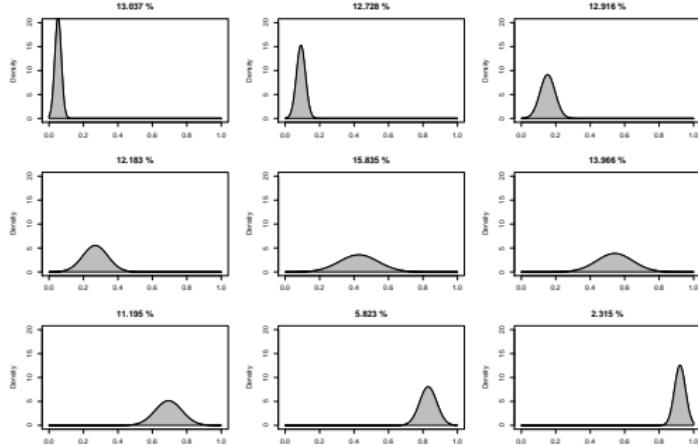
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- Can accurately characterize the methylation densities using a kernel mixture model
- Key idea: use the same kernels across the sites & groups but allow the weights to vary
- SHARed Kernel (SHARK) method (*Lock & Dunson, 2015*)**

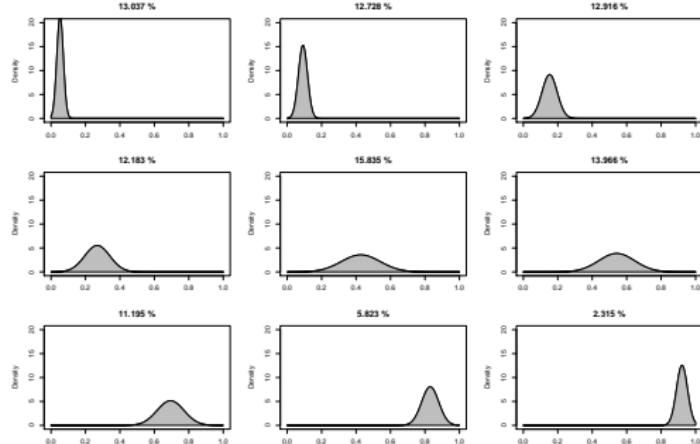
Shark - some details



• The methylation density at site j in group g is f_{jg} :

$$f_{jg}(y) = \sum_{h=1}^k \pi_{jgh} \mathcal{K}(y; \theta_h)$$

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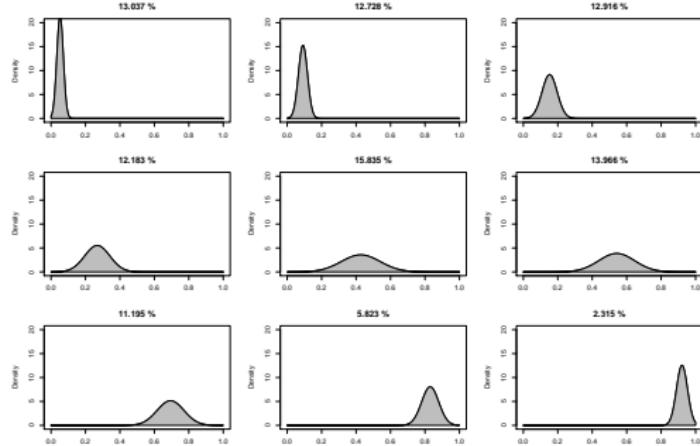


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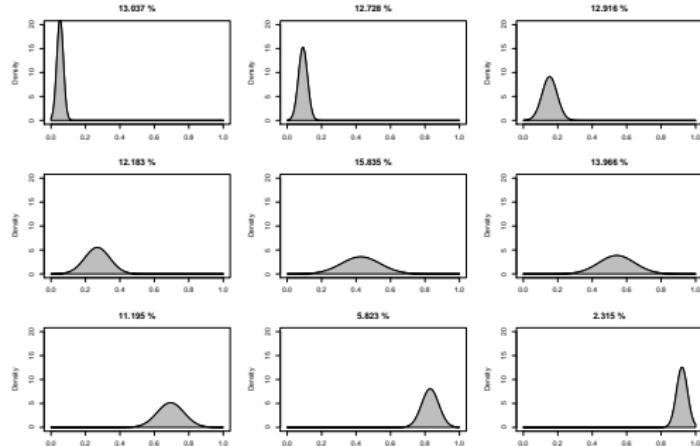


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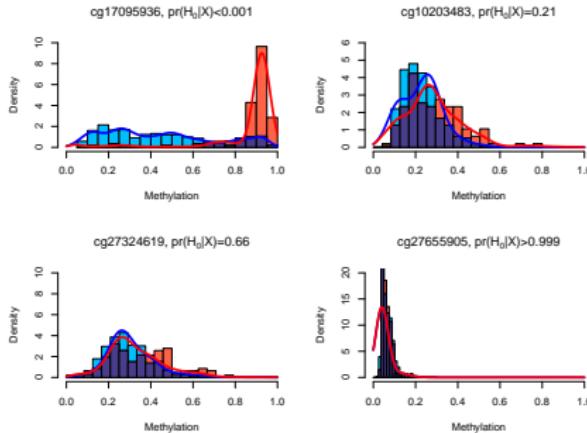


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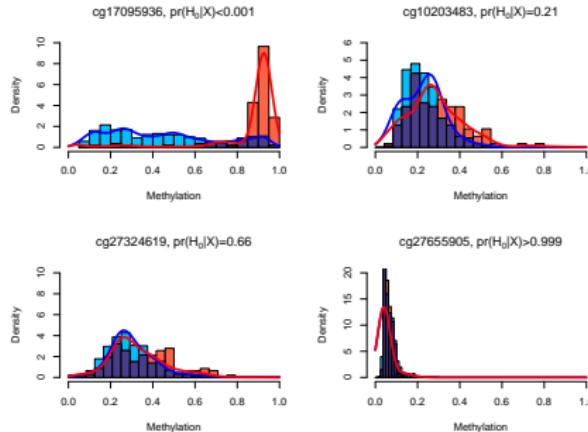
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Shark - implementation (continued)



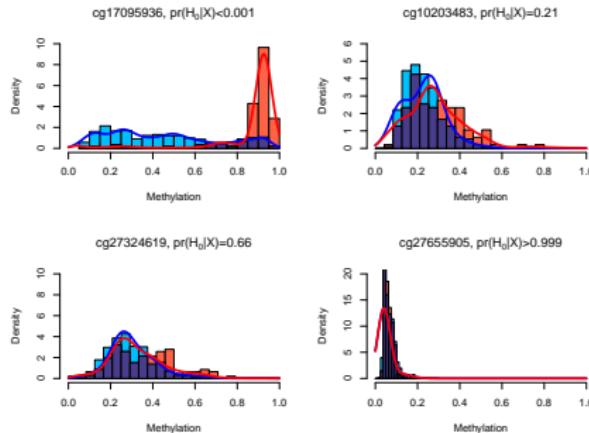
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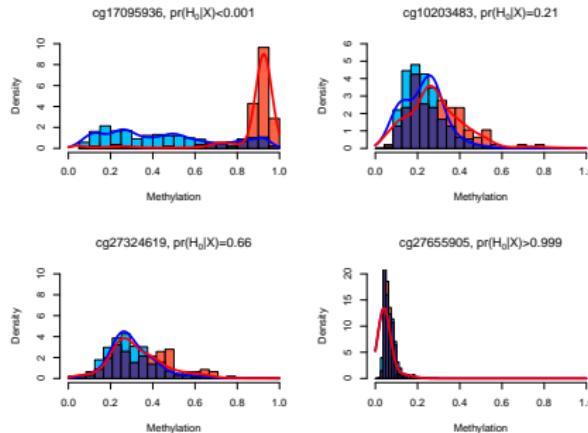
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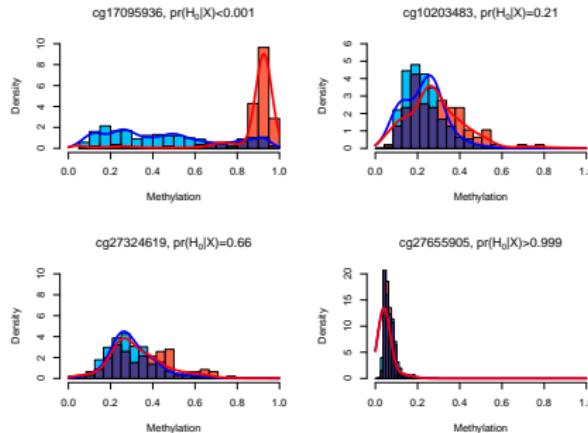
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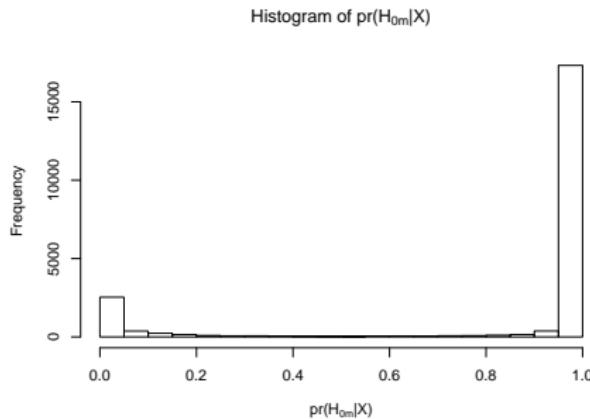
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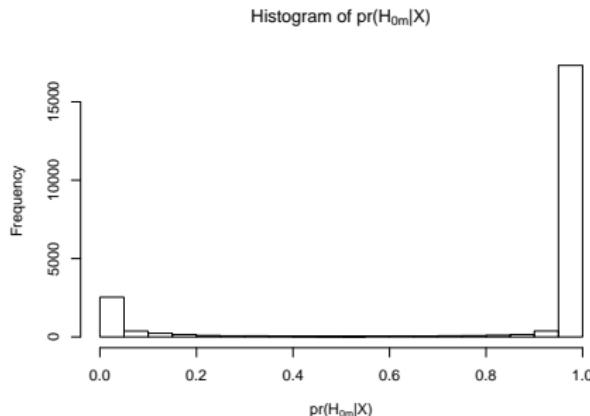
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Results for Cancer Genome Atlas Data



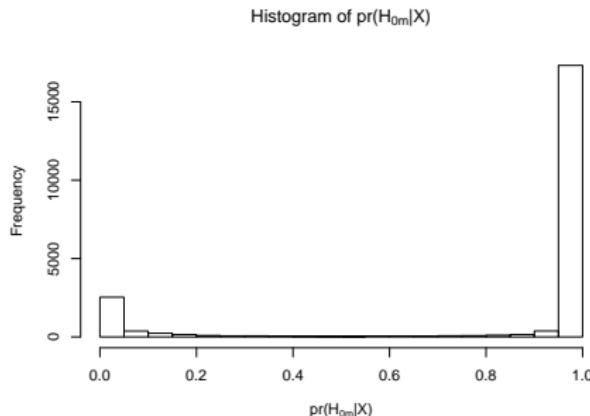
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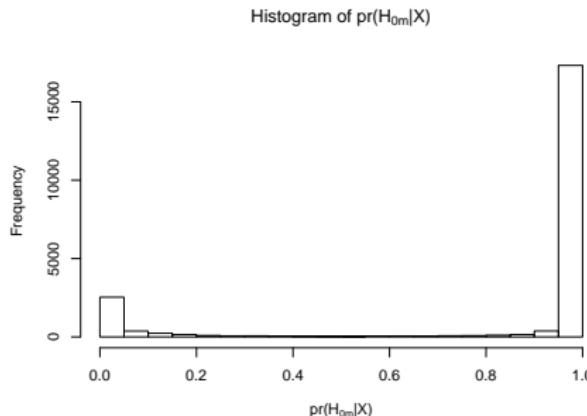
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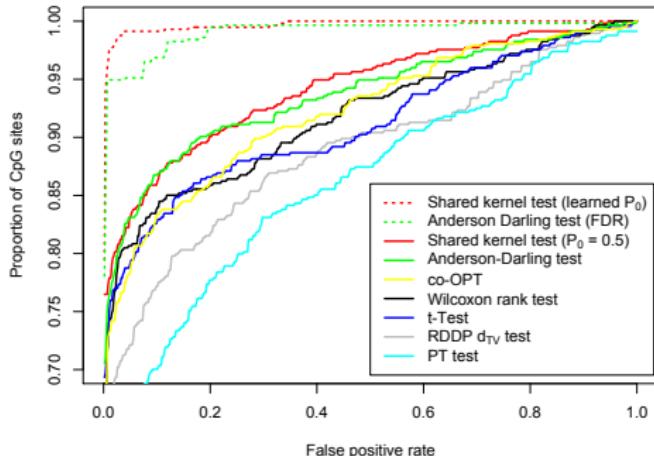
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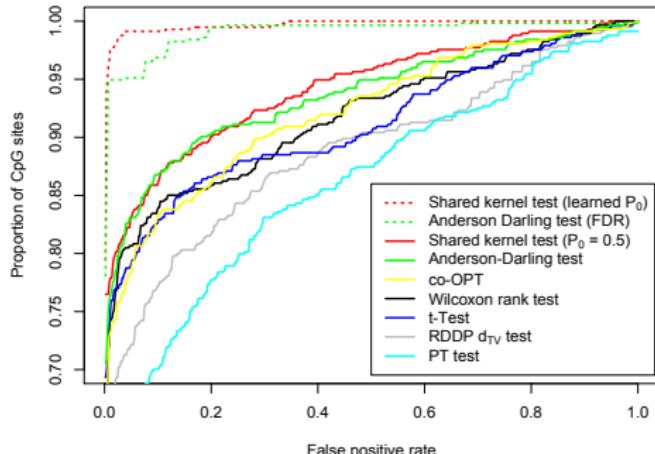
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Discussion & Comparisons



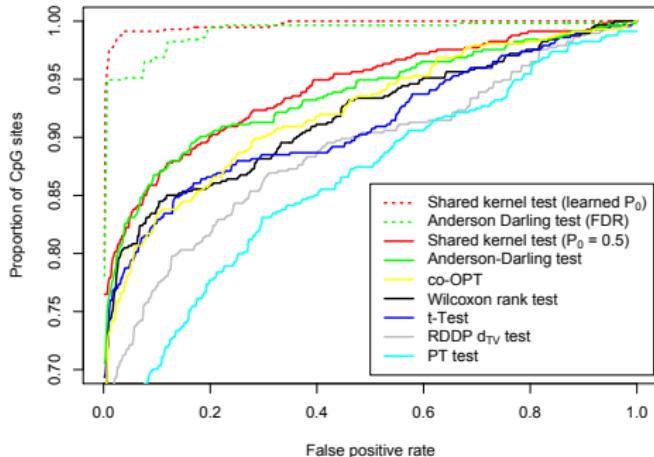
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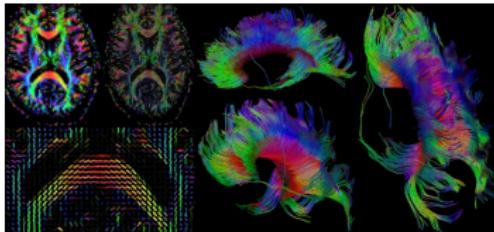
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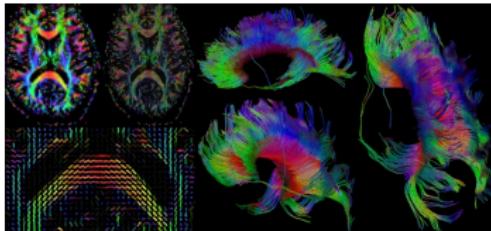
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- ✿ We compared power of our approach with alternatives

Shared kernel testing for complex phenotypes



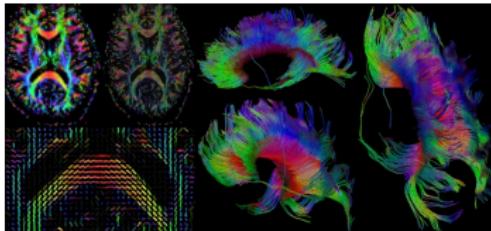
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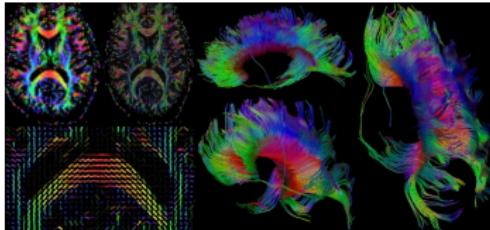
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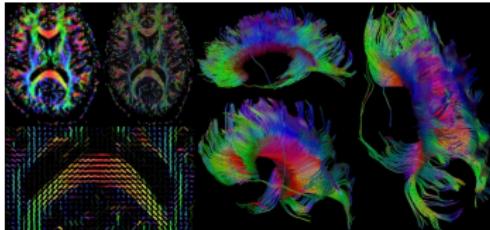
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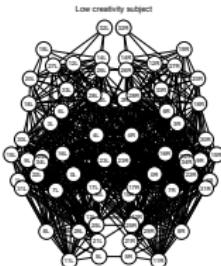
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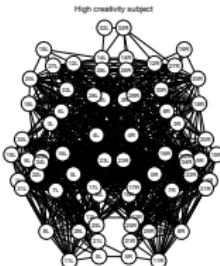
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- Then, $X_{i[u,v]} = 1$ if there is any connection between regions u & v for individual i , and $X_{i[u,v]} = 0$ otherwise

A nonparametric model of variation in brain networks



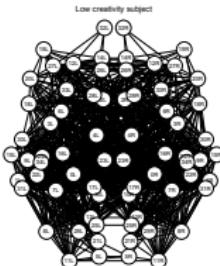
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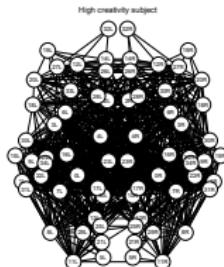
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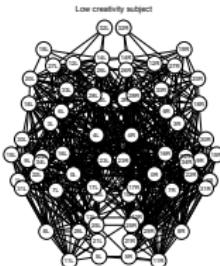


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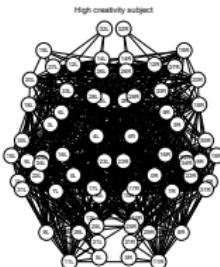


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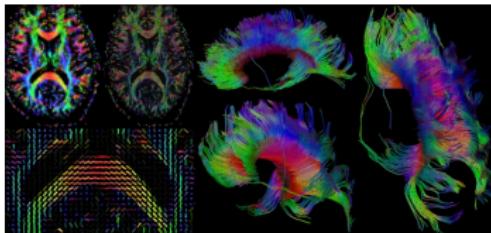


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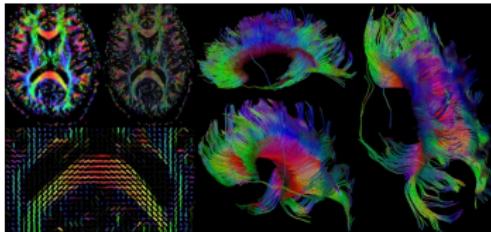
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Bayesian inferences



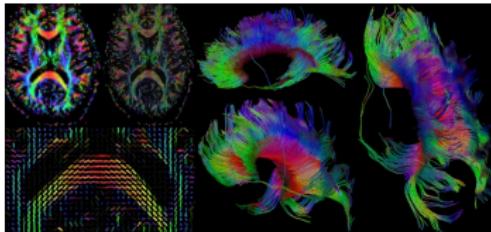
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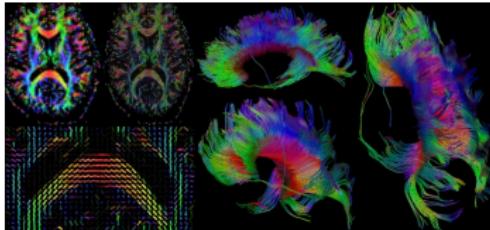
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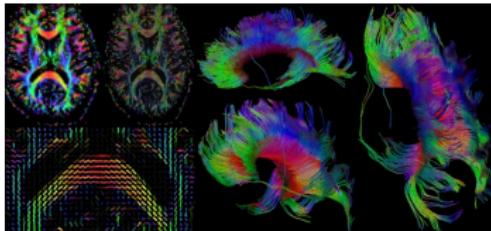
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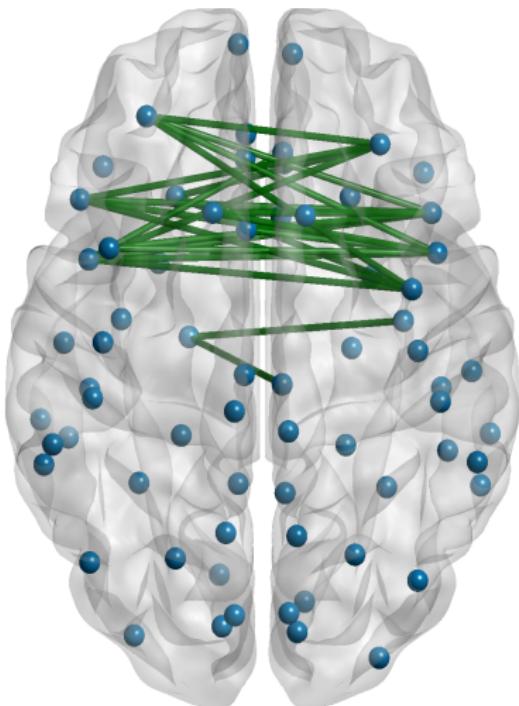
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- **Adjusts for multiple testing reducing false positives**

Application to creativity

Results from local testing

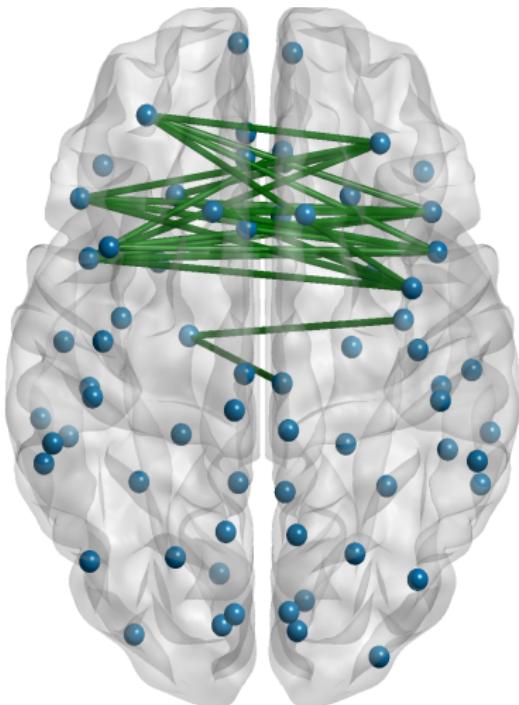


High-dimensional data (big p)

- Apply model to brain networks of 36 subjects (19 with high creativity, 17 with low creativity—measured via CCI).

Application to creativity

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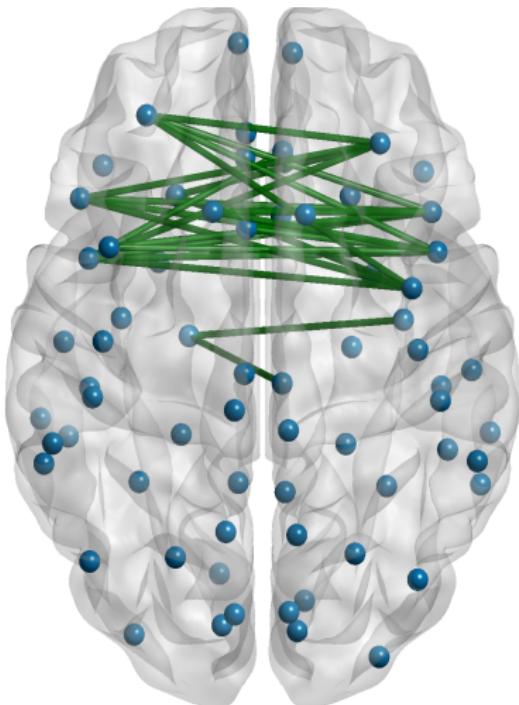


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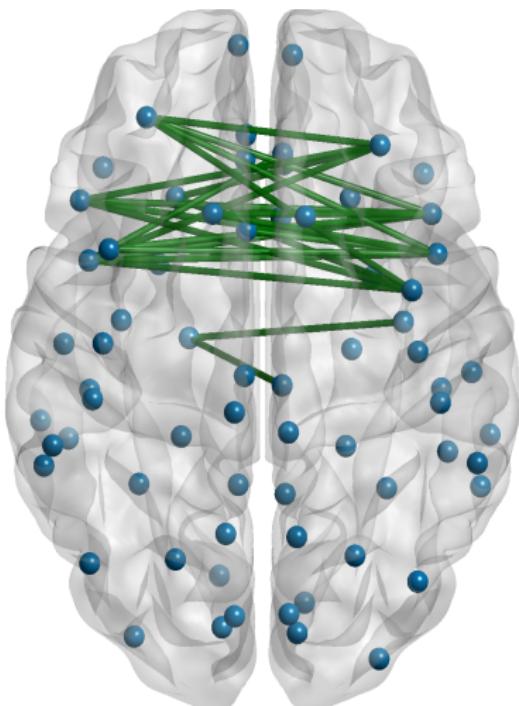


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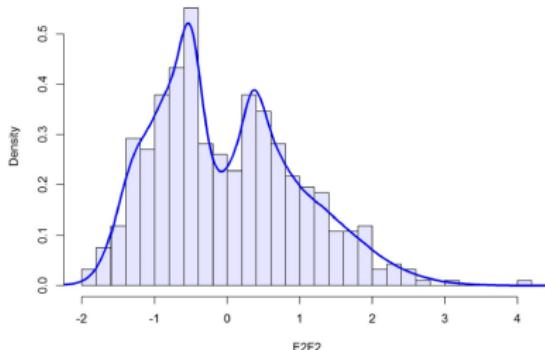
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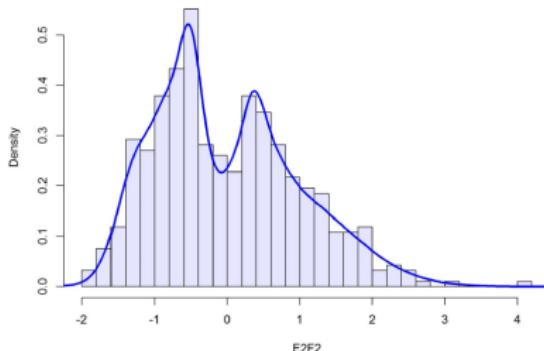
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MOBS - comments



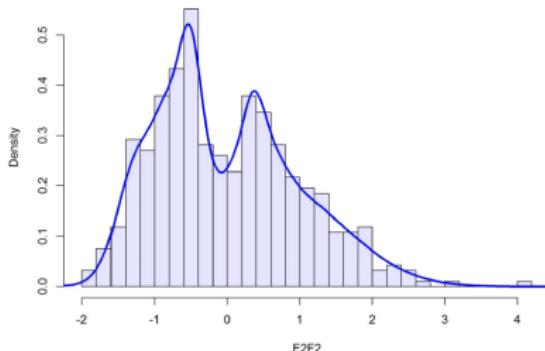
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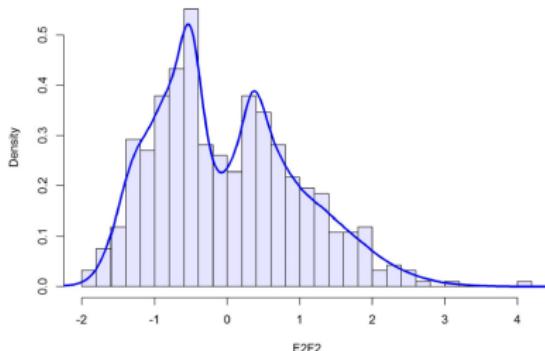
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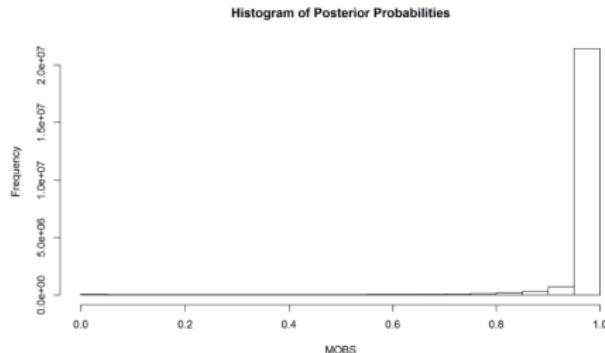
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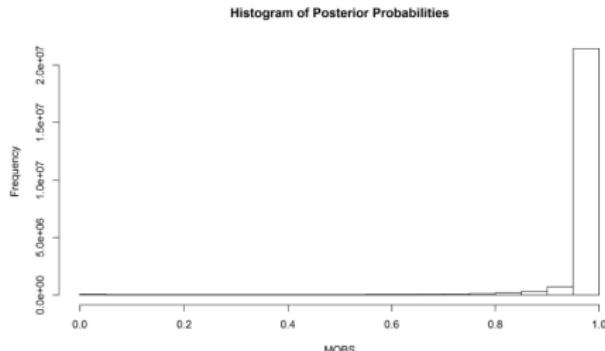
- Algorithm is very fast & scalable to huge p + trivially parallelizable
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- Competitive with the state of the art in performance
- Particularly good at detecting complex distributional changes

Application to cis-eQTL data



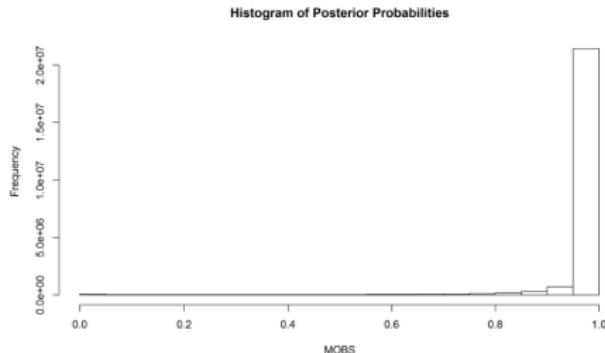
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Application to cis-eQTL data



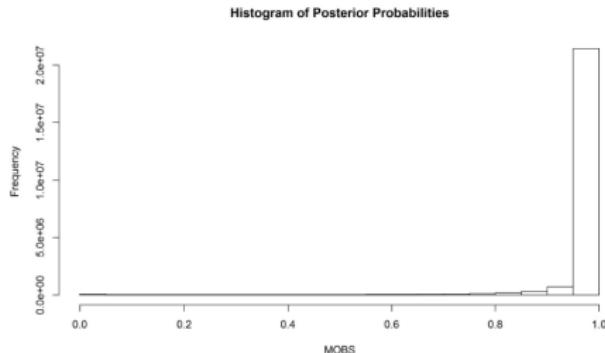
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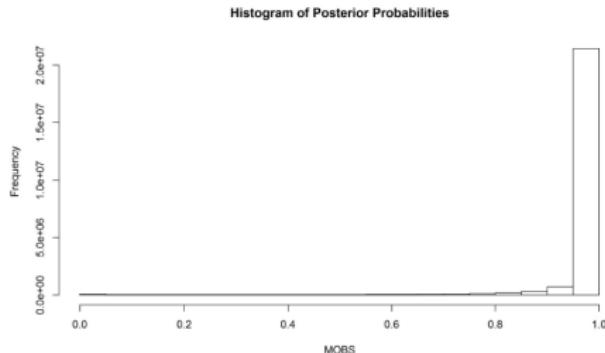
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- 38 million Single Nucleotide Polymorphisms (SNPs)
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Application to cis-eQTL data



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- 0.4% of $\text{pr}(H_0j) < 0.05$ - picking up differences in distribution other methods miss

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- There is a very rich literature & increasing focus on scalability
- One important direction is to obtain methods for assessing when we are attempting inferences on too fine of a scale for our data
- Ideally can then automatically coarsen the scale to answer solvable questions - e.g., Peruzzi & Dunson (2018)

Some references - large n Bayes

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- ✿ Also useful to take a step away from the fully Bayes framework by using modularization, composite likelihoods, c-Bayes, etc
- ✿ Such generalized Bayes methods can have improved computational performance & robustness