

Scalable Bayesian Inference

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Duke
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Outline

Motivation & background

Big n

High-dimensional data (big p)

Typical approaches to 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
- Algorithms scalable to huge data - potentially using many computers

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



Bayes approaches

- ✳ Bayesian methods offer an attractive general approach for modeling complex data



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

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- Often θ is moderate to high-dimensional & the integral in denominator is intractable
- Hence, in interesting models the posterior is not available analytically - what to do??

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$$\pi_n(\theta|Y^{(n)}) \approx N(\hat{\mu}_n, \Sigma_n)$$

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

Alternative analytic approximations

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

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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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 2. **Accept proposal by letting $\theta^{(t)} = \theta^*$ with probability**

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

Comments on MCMC & MH in particular

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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

MCMC & Computational bottlenecks



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MCMC & Computational bottlenecks



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- ☛ Can also increase with the sample size n
- ☛ 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**

MCMC - A potential 2nd bottleneck

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- ✎ “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

MCMC: Causes of scalability problems

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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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- ✎ Some popular algorithms have been shown to not be scalable while others can be made scalable
- ✎ 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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Some Solutions

- ✿ **Embarrassingly parallel (EP) MCMC**: run MCMC in parallel for different subsets of data & combine.

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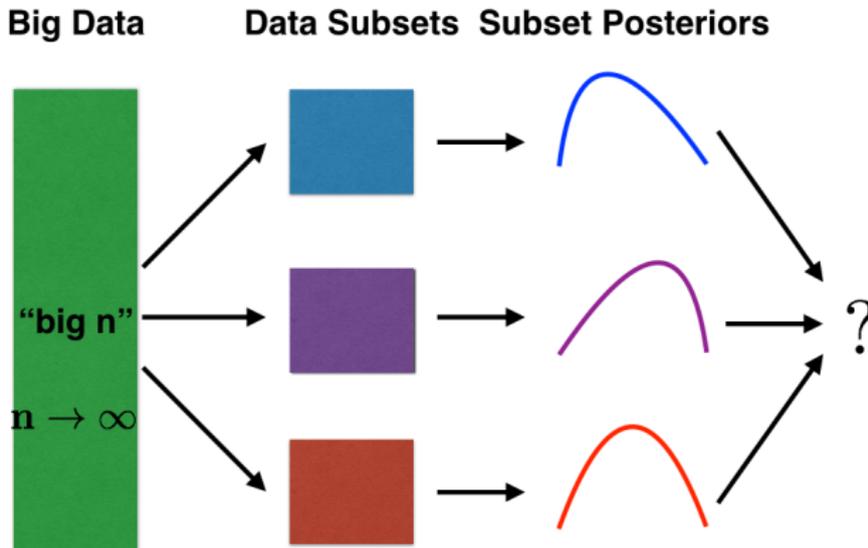
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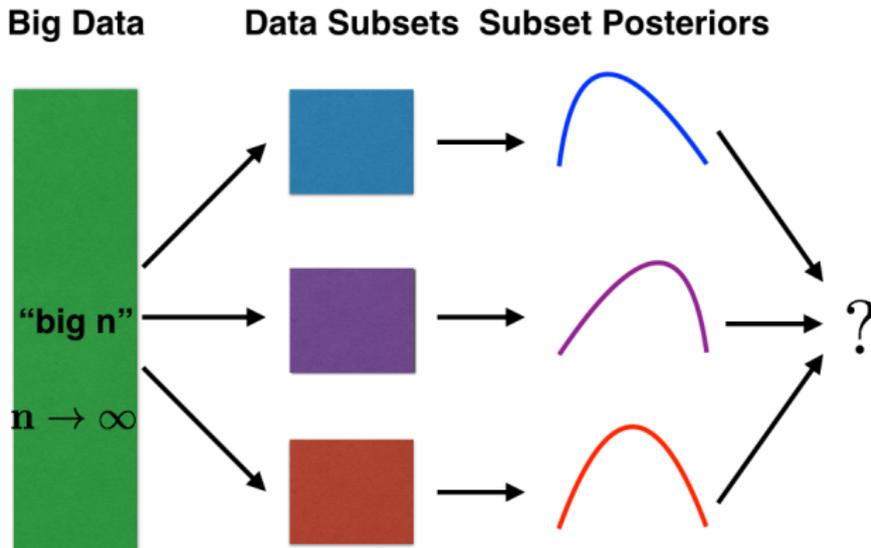
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- ☞ **C-Bayes**: Condition on observed data being in small neighborhood of data drawn from assumed model [*ROBUST*]
- ☞ **Hybrid algorithms**: run MCMC for a subset of the parameters & use a fast estimate for the others.

Embarrassingly parallel MCMC



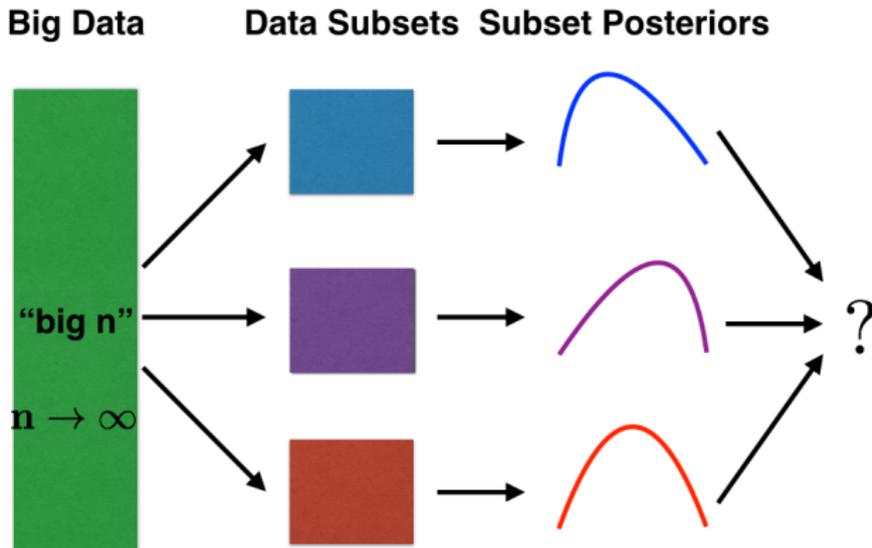
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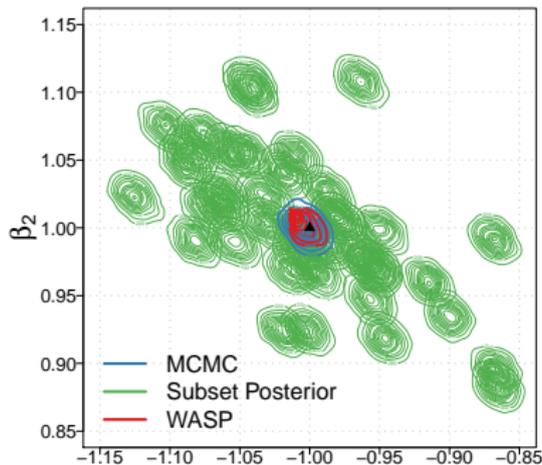
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Embarrassingly parallel MCMC



- ✎ Divide large sample size n data set into many smaller data sets stored on different machines
- ✎ Draw posterior samples for each subset posterior in parallel
- ✎ **‘Magically’ combine the results quickly & simply**

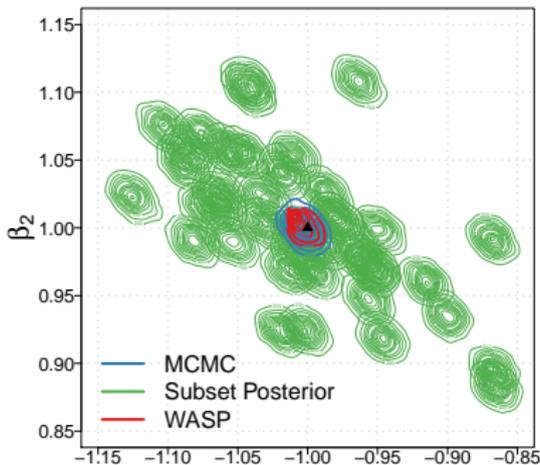
Toy Example: Logistic Regression



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

Subset posteriors: 'noisy' approximations of full data posterior.

Toy Example: Logistic Regression



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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 $Y^{(n)}$

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

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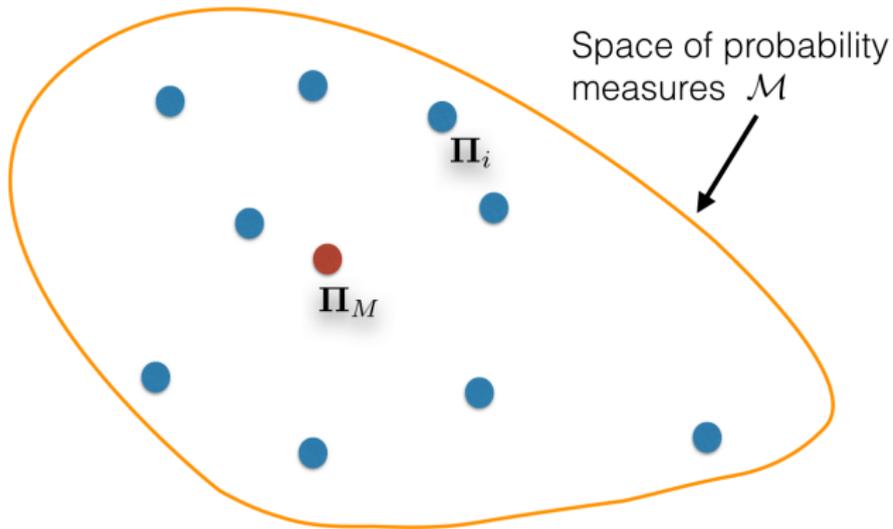
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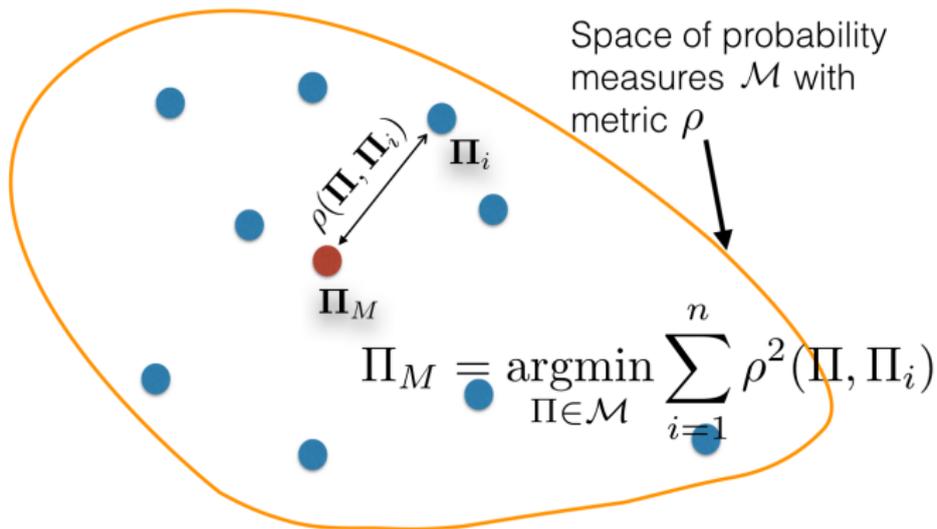
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Barycenter in Metric Spaces



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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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- ✎ 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

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

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- ✿ **Approximate kernel in exact chain with more computationally tractable alternative**

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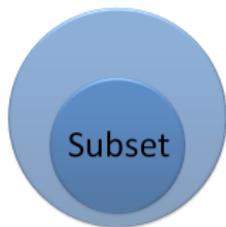
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- ✎ **Often larger approximation error \rightarrow larger s_ϵ & rougher approximations are better when speed super important**

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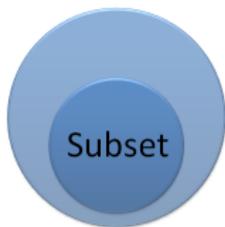


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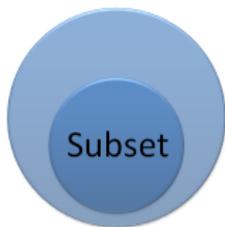
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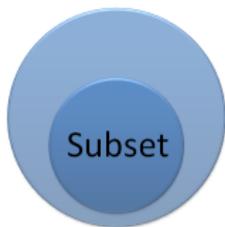
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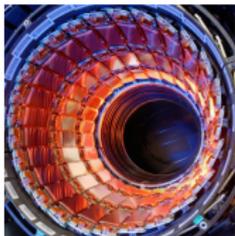
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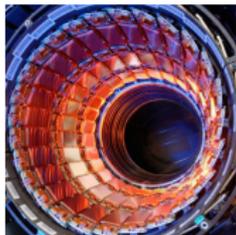
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- ☛ **Assumptions hold with high probability for subsets $>$ minimal size (wrt distribution of subsets, data & kernel).**

Application to SUSY dataset



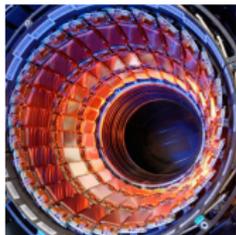
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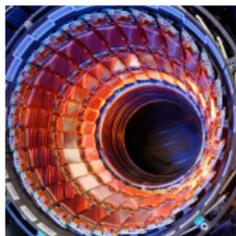


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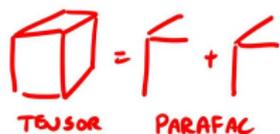
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Application 2: Mixture models & tensor factorizations

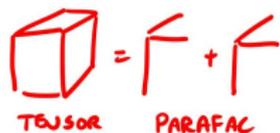


☛ We also considered a nonparametric Bayes model:

$$\text{pr}(y_{i1} = c_1, \dots, y_{ip} = c_p) = \sum_{h=1}^k \lambda_h \prod_{j=1}^p \psi_{hc_j}^{(j)},$$

a very useful model for multivariate categorical data

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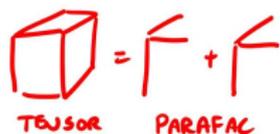
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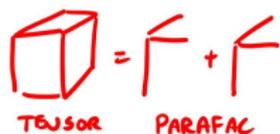
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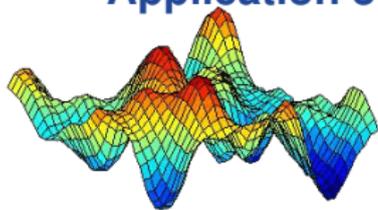
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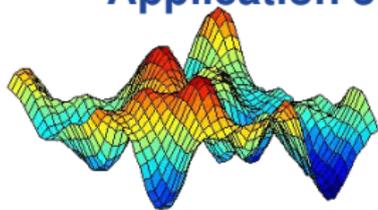
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Application 3: Low rank approximation to GP



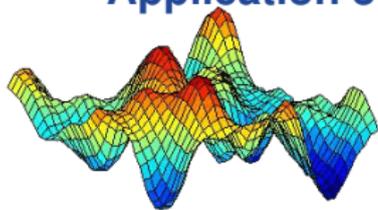
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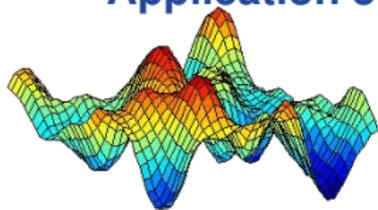
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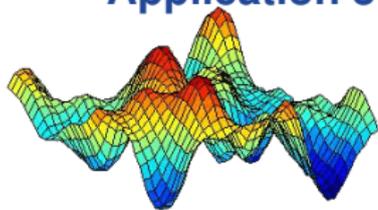
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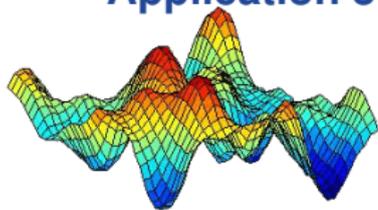
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- ✿ Robustness: one topic we haven't discussed yet is robustness

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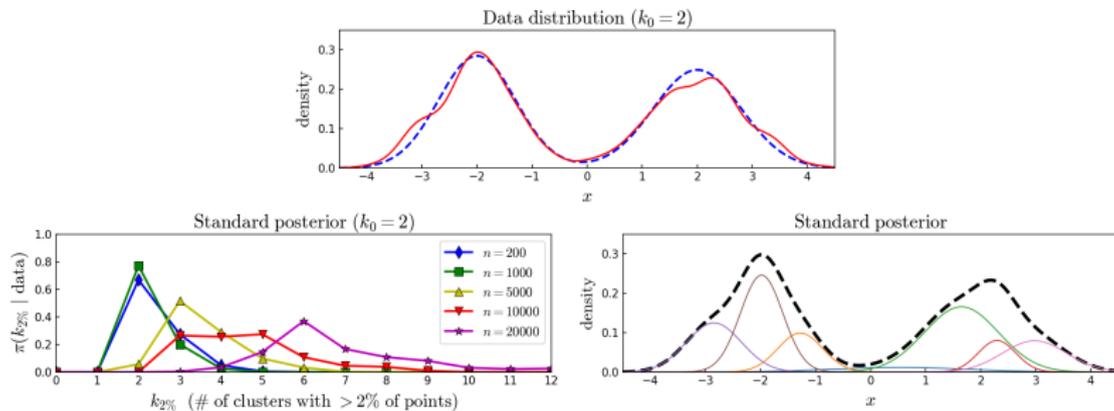
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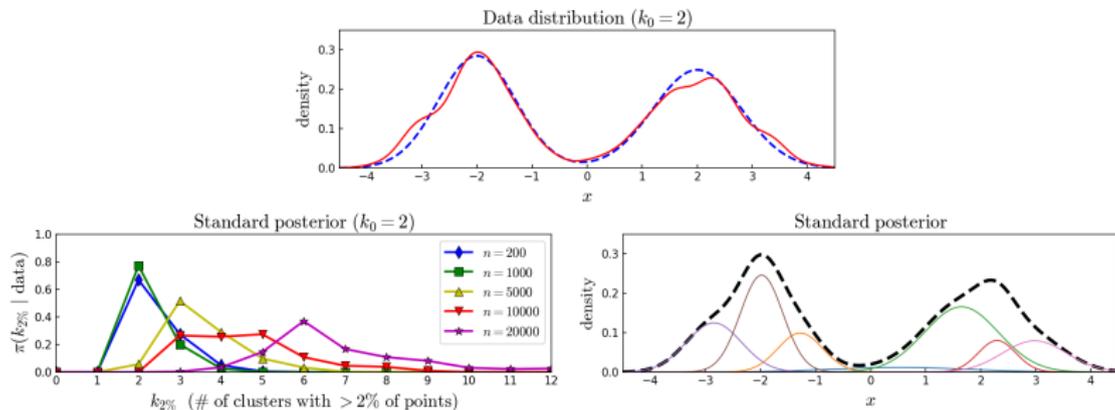
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- ✎ **Appealing to tweak Bayesian paradigm to be inherently more robust**

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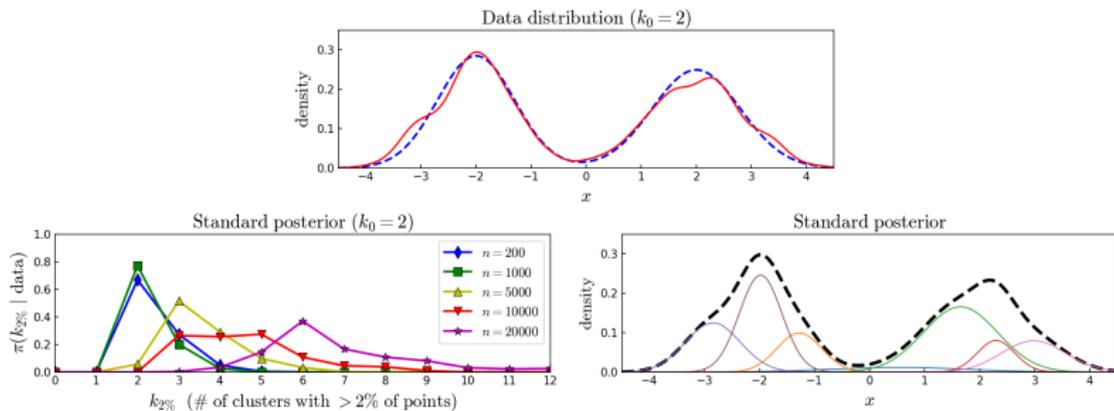
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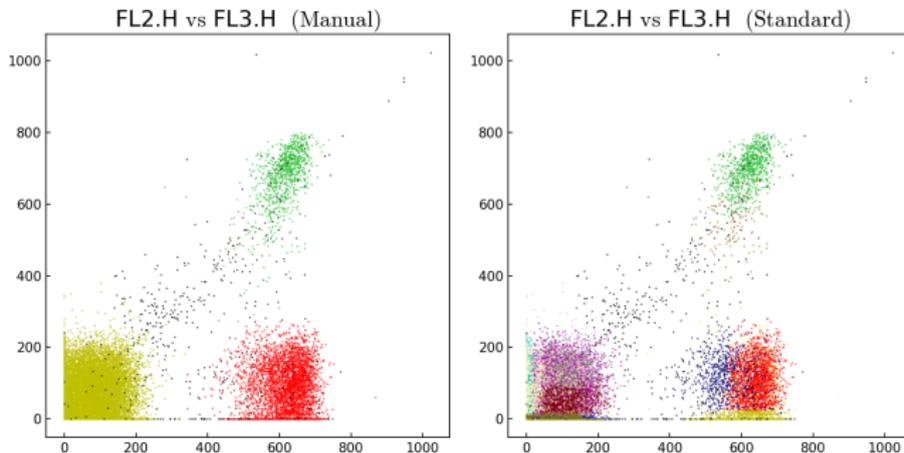
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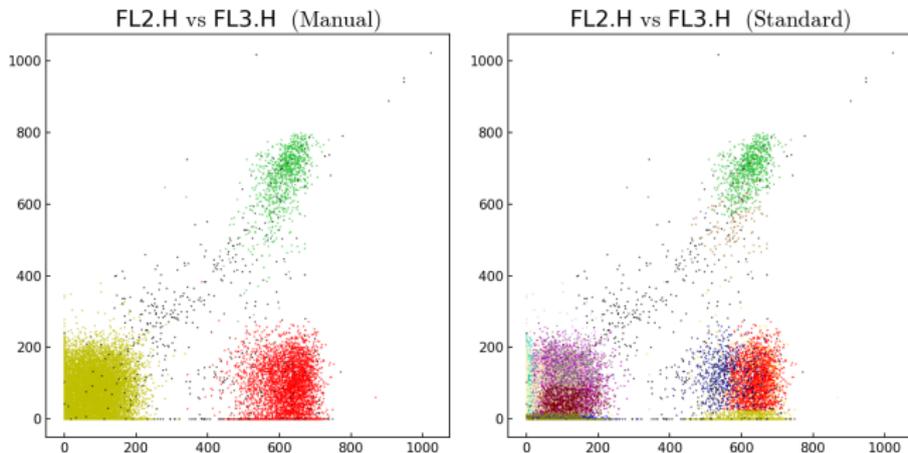
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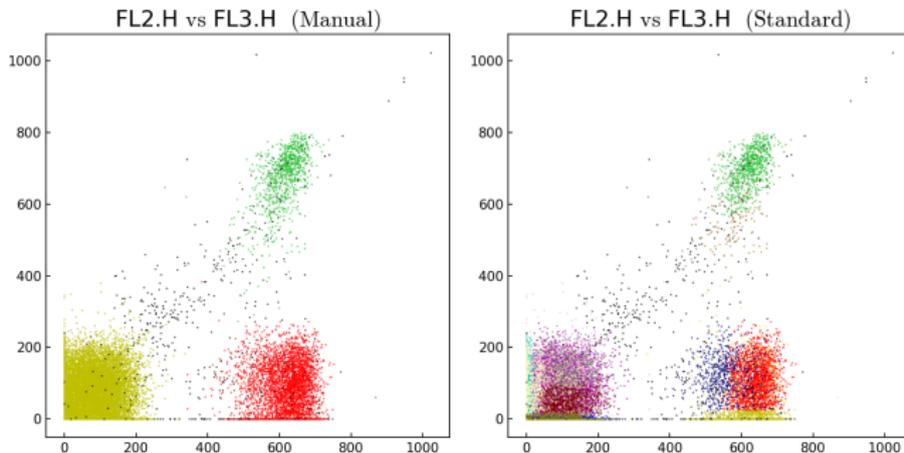
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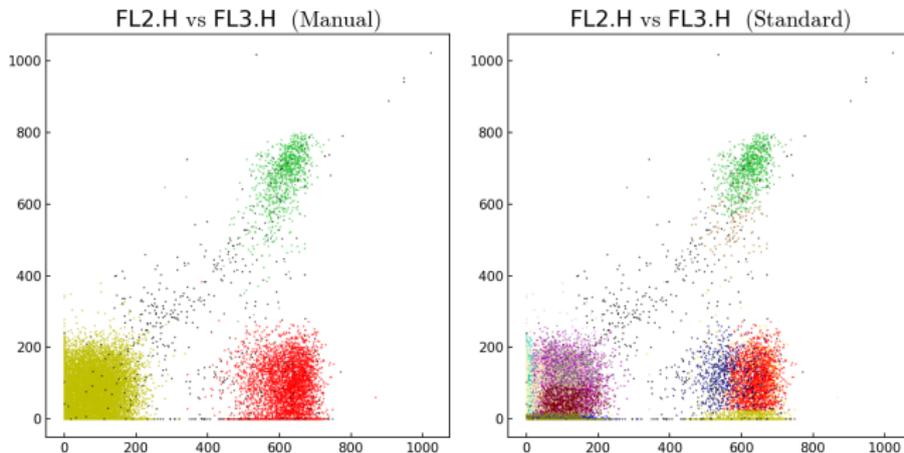
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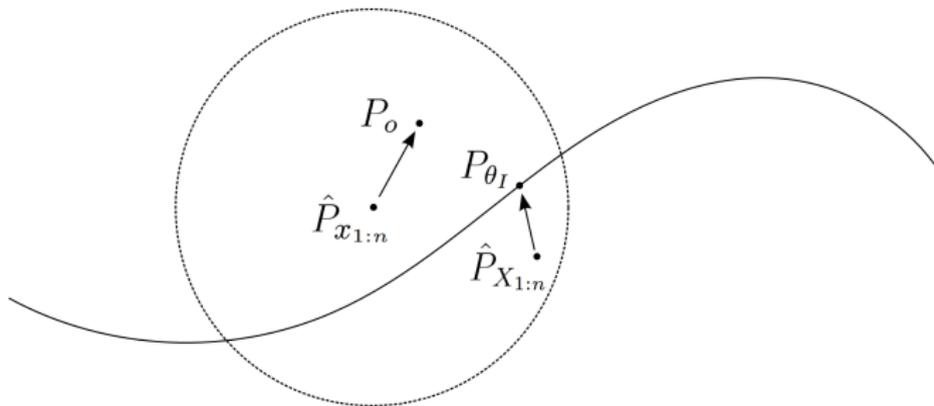
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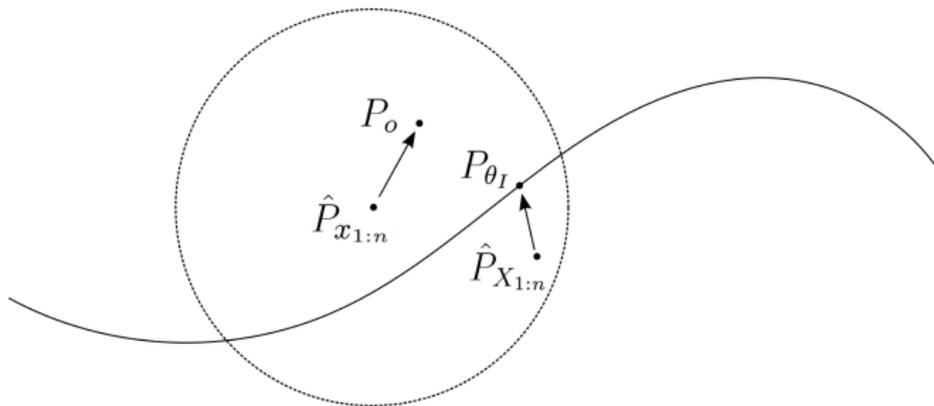
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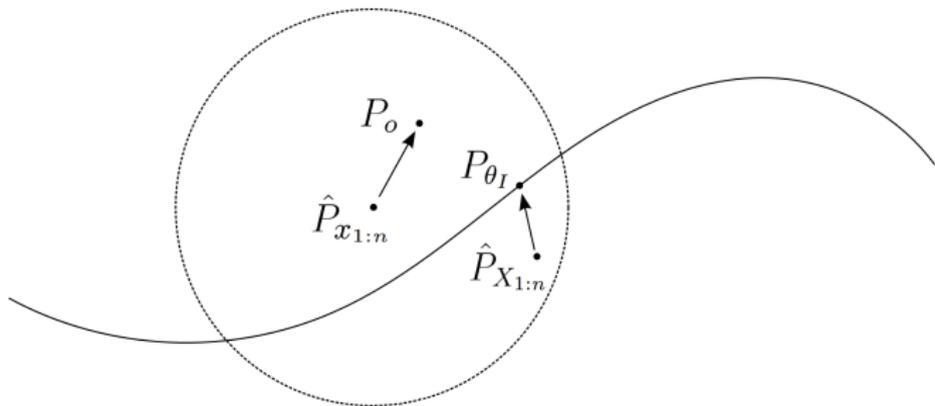
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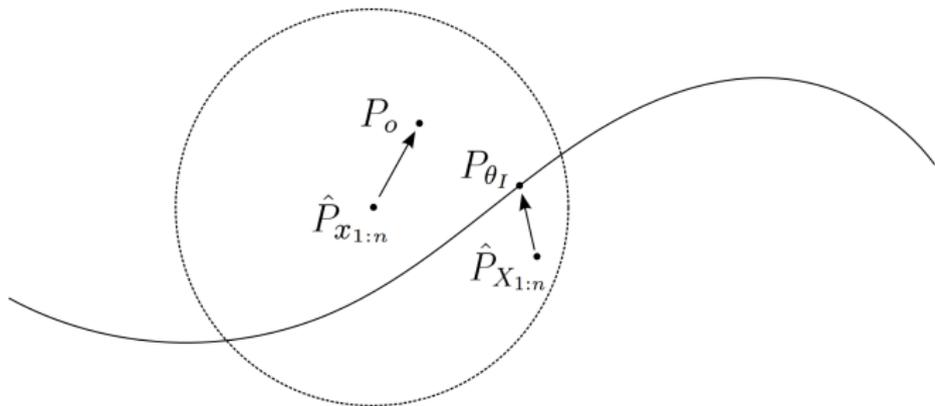
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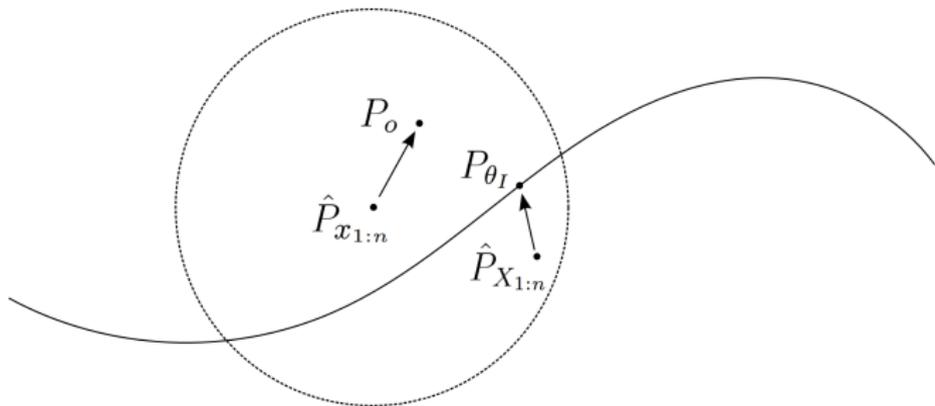
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- ✎ Suppose X_1, \dots, X_n i.i.d. $\sim P_{\theta_I}$ are unobserved *idealized data*.
- ✎ However, the *observed data* x_1, \dots, x_n are actually a slightly corrupted version of X_1, \dots, X_n in the sense that $d(\hat{P}_{X_{1:n}}, \hat{P}_{x_{1:n}})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

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- ✎ **More generally, consider**

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

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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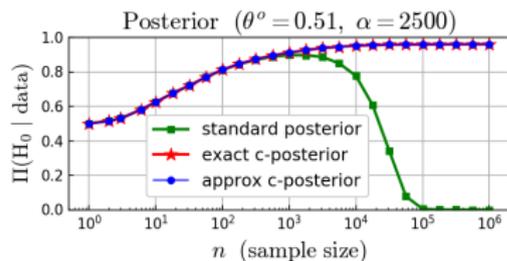
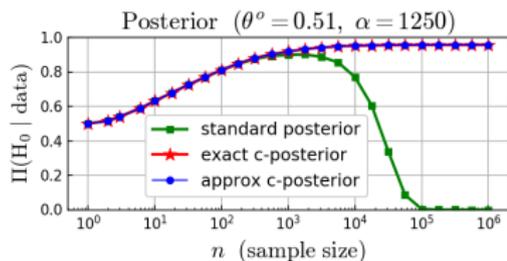
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- ☛ The c-posterior is robust to this, but the standard posterior is not.



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- ☛ Model: $X_1, \dots, X_n | w, \varphi$ i.i.d. $\sim \sum_{i=1}^K w_i f_{\varphi_i}(x)$
- ☛ Prior: $w \sim \text{Dirichlet}(\gamma_1, \dots, \gamma_K)$ and $\varphi_1, \dots, \varphi_K \stackrel{iid}{\sim} H$.
- ☛ c-Posterior is approximated as

$$\pi(w, \varphi | d_n(X_{1:n}, x_{1:n}) < R) \propto \pi(w, \varphi) \prod_{j=1}^n \left(\sum_{i=1}^K w_i f_{\varphi_i}(x_j) \right)^{\zeta_n}$$

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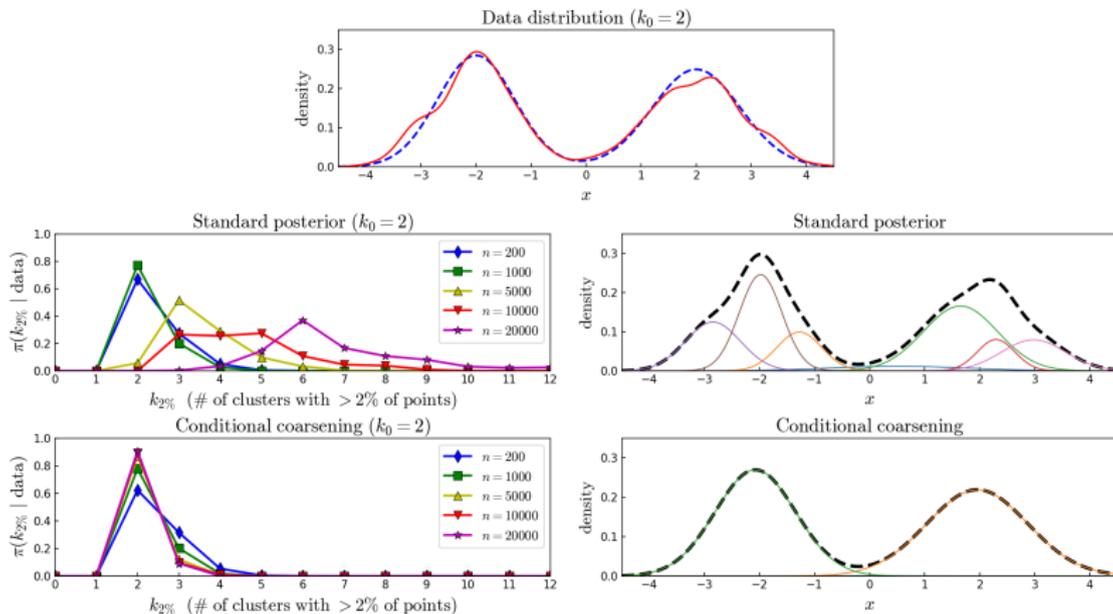
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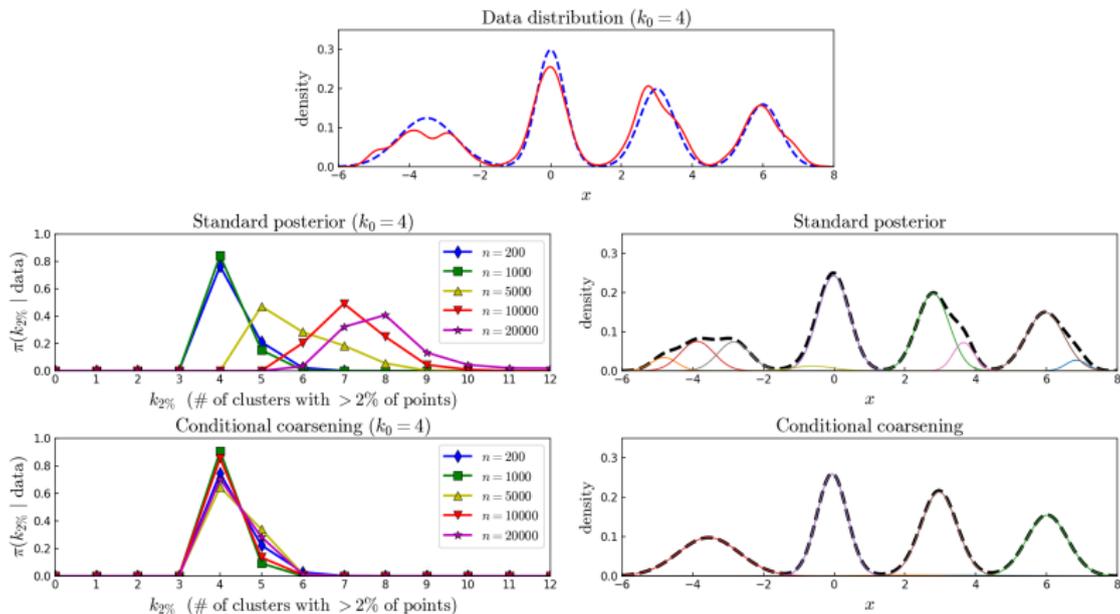
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- ☛ A straightforward MCMC algorithm can be used for computation
- ☛ Scales well to large datasets
- ☛ EP-MCMC, a-MCMC etc can be used to enhance scalability

Example: Perturbed mixture of Gaussians

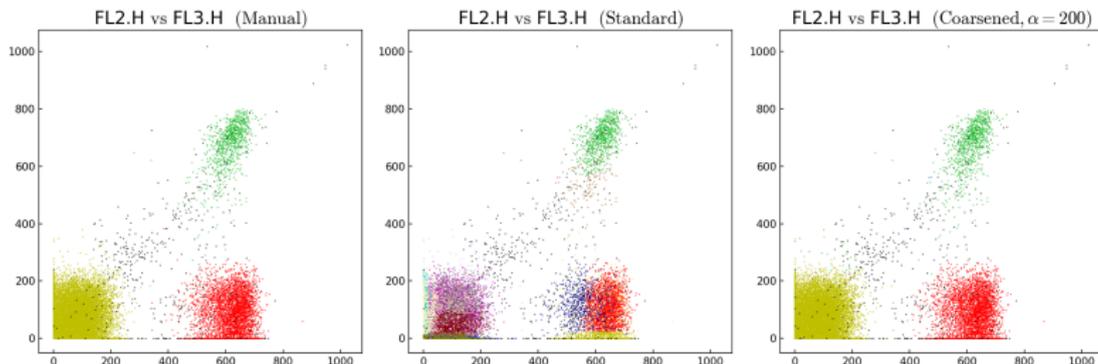


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Results: Flow cytometry clustering

Clustering on test datasets closely matches manual ground truth.



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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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- ✎ c-Bayes can be implemented with a particular power posterior
- ✎ All the scalable MCMC tricks developed for regular posteriors can be used directly
- ✎ 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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- ✎ **Scalable, excellent mixing & empirical/predictive performance**

Outline

Motivation & background

Big n

High-dimensional data (big p)

Scaling Bayes to high-dimensional data

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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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- ☞ Choose p-value threshold controlling False Discovery Rate (FDR) - eg Benjamini-Hochberg (BH)
- ☞ **Get a list of discoveries & hopefully run follow-up studies to verify**

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- ☞ **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

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$$\begin{aligned}\tilde{\beta} &= \operatorname{argmin}_{\beta} \sum_{i=1}^n (y_i - x_i' \beta)^2 + \lambda \sum_{j=1}^p \beta_j^2 \\ &= \operatorname{argmin}_{\beta} \|Y - X\beta\|_2^2 + \lambda \|\beta\|_2^2.\end{aligned}$$

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- ☛ Dual interpretation as a Bayesian estimator under a Gaussian prior centered at zero & a least squares estimator with a penalty on large coefficients
- ☛ 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

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

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

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- ☛ $\tilde{\beta}$ is sparse & contains exact zeros values

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

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- ☛ **Datta & Dunson (20)16, *Biometrika*) - develop such approaches for huge dimensional sparse count data arising in genomics**

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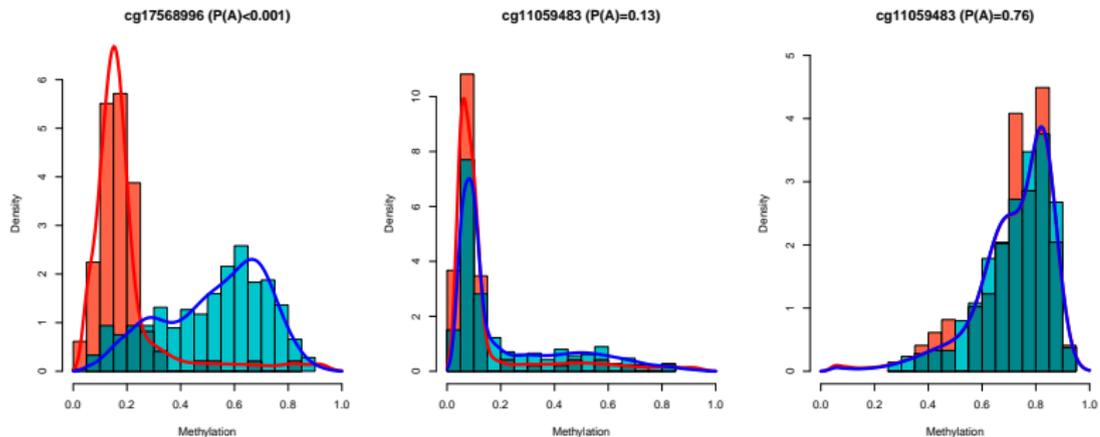
Features of a Bayesian approach

- ✿ Bayesian approach provides a full posterior $\pi(\beta|Y, X)$ characterizing uncertainty instead of just a sparse point estimate $\hat{\beta}$
- ✿ By using MCMC, we can easily get credible bands (Bayesian confidence intervals) for not only the β_j 's but also for any functional of interest
- ✿ Relatively straightforward to incorporate extensions to allow hierarchical dependence structures, multivariate responses, missing data, etc
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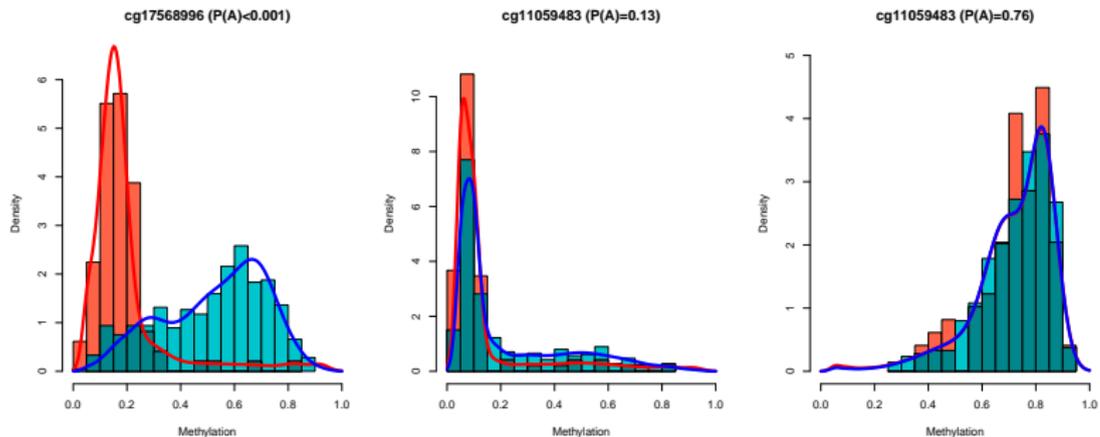
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 3. provide a way to deal with intractable $p \gg n$ problems

Application 1: DNA methylation arrays



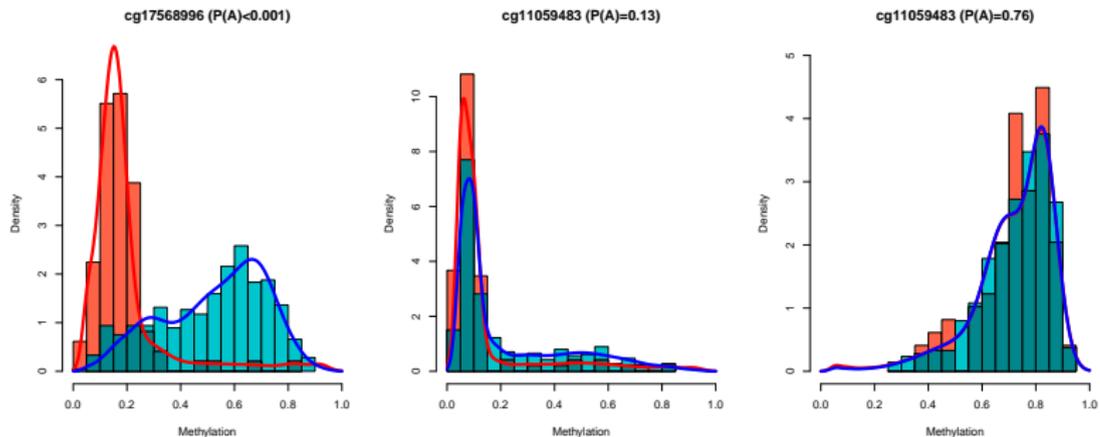
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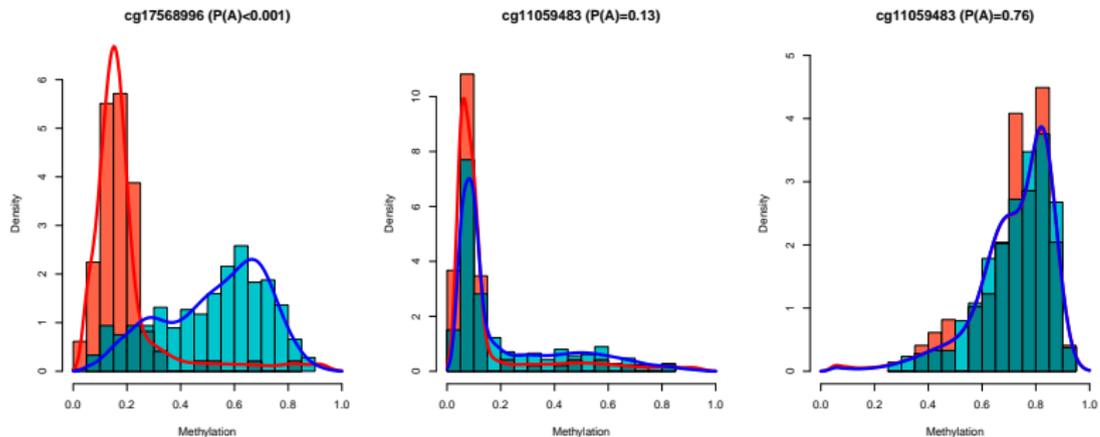
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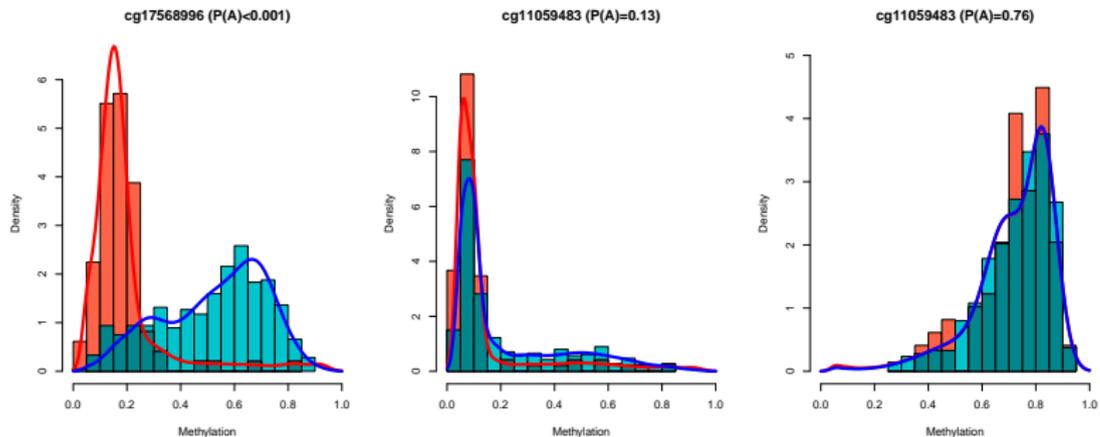
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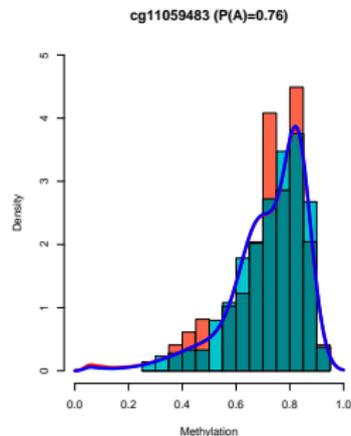
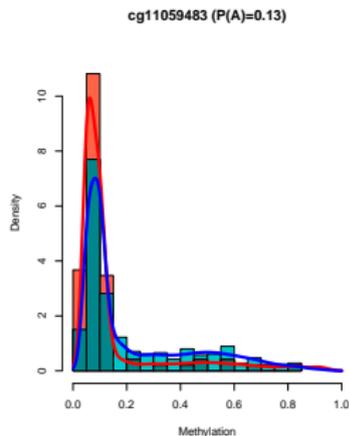
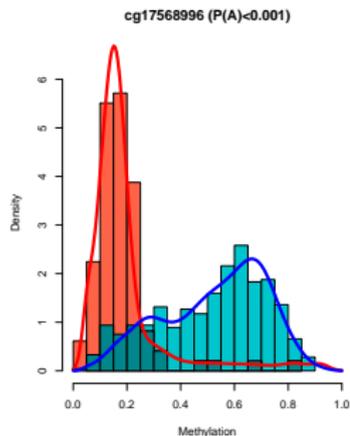
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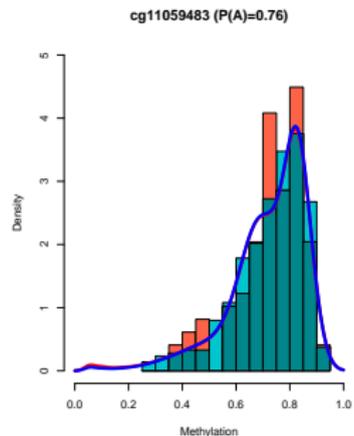
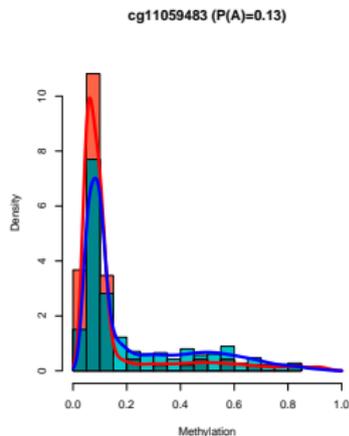
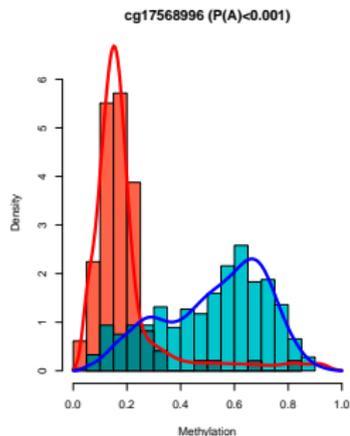
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- ☞ Measurements in $[0,1]$ interval, ranging from no methylation to fully methylated
- ☞ Representative data from the Cancer Genome Atlas
- ☞ **Clearly distributions exhibit multimodality & skewness**

Comments



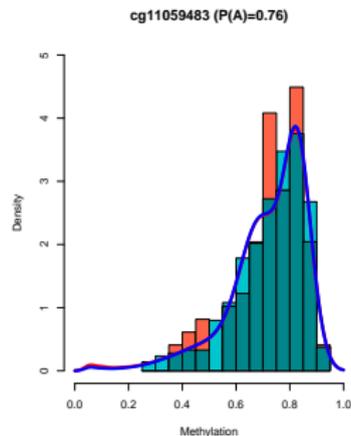
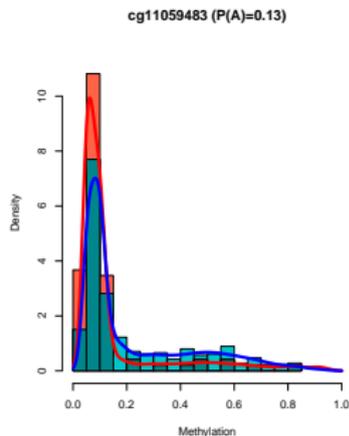
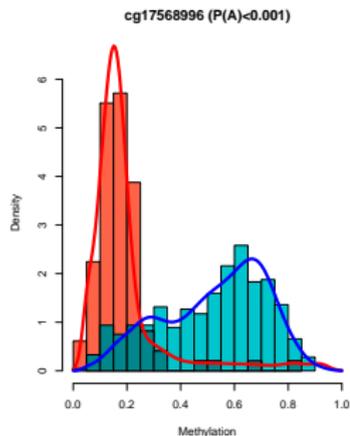
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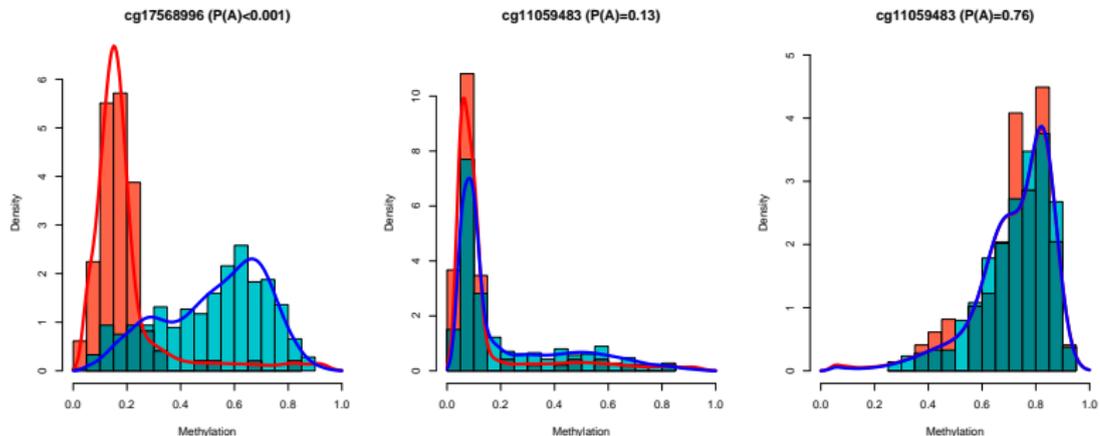
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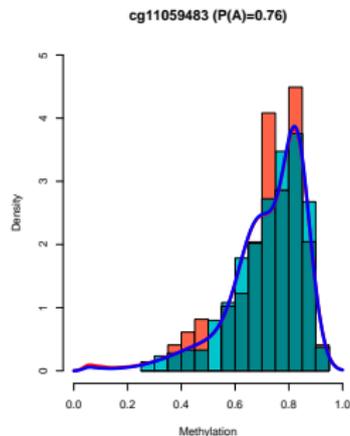
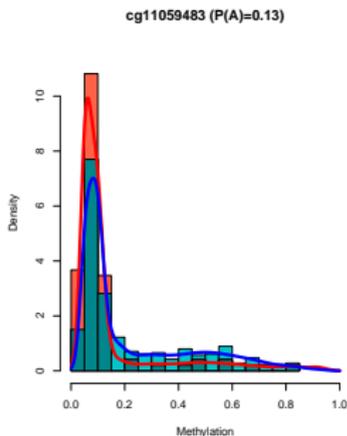
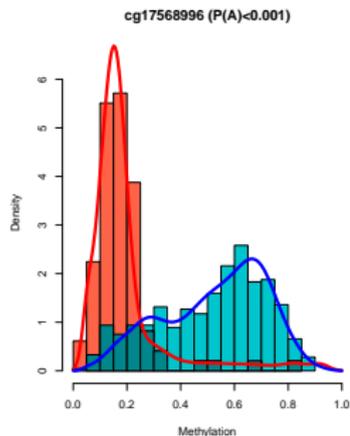
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Comments



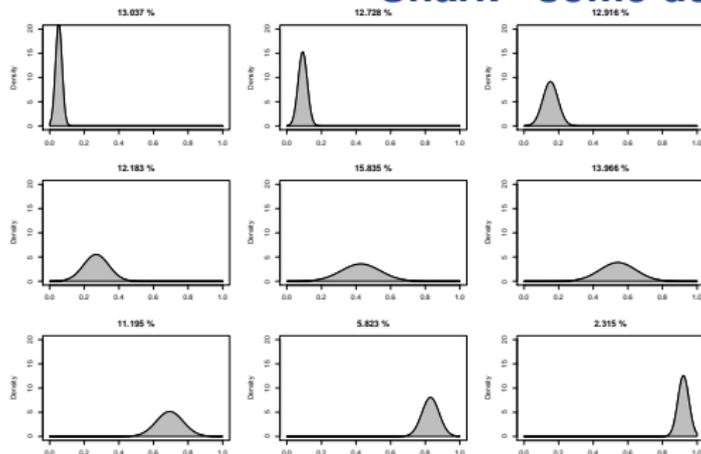
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- ☞ Key idea: use the same kernels across the sites & groups but allow the weights to vary
- ☞ **SHARed Kernel (SHARK) method (Lock & Dunson, 2015)**

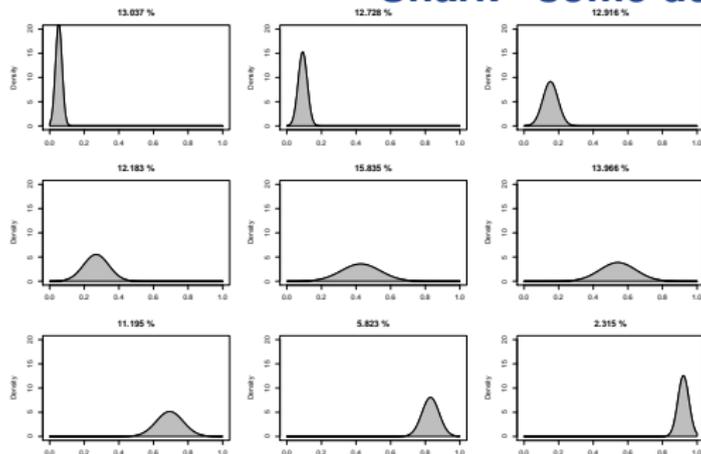
Shark - some details



🐋 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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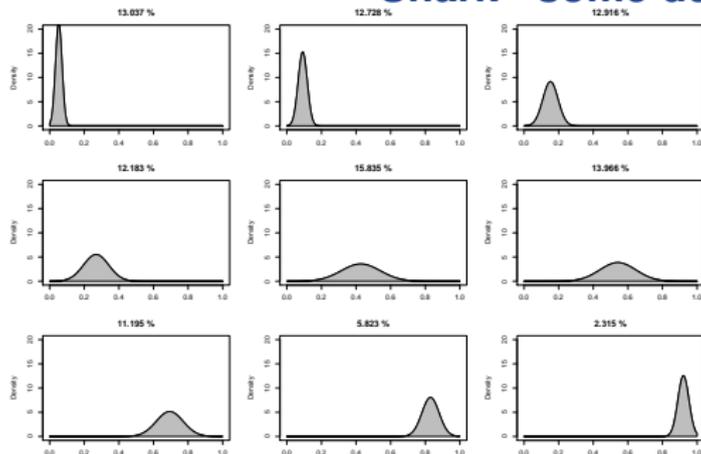


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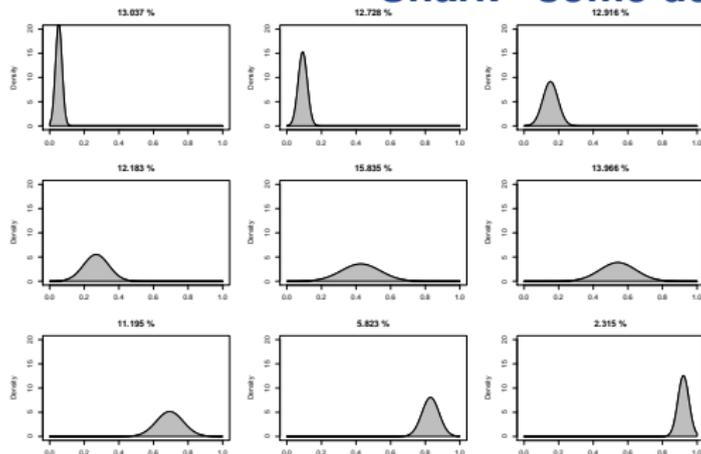
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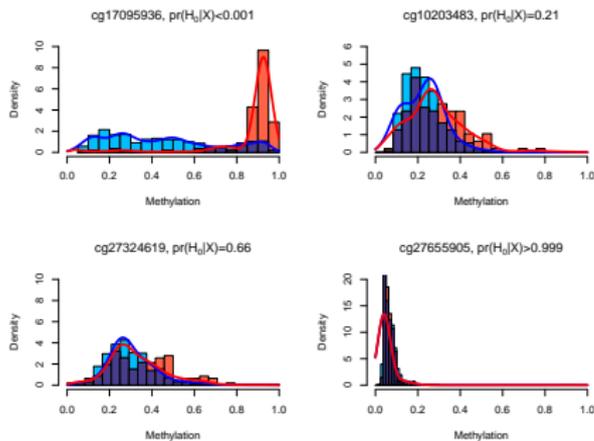


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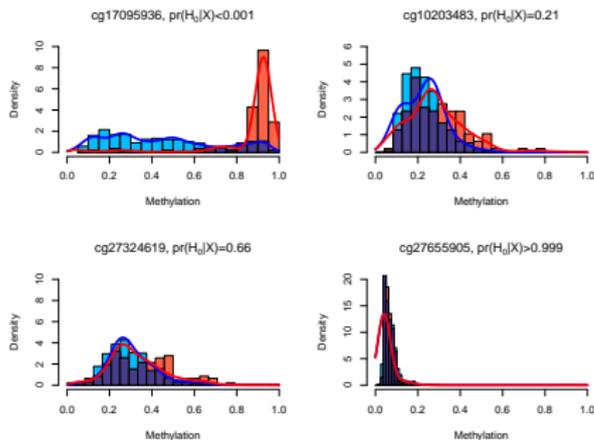
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- ☛ $\mathcal{K}(y; \theta_h)$ is a *shared* kernel (truncated normal in this case)
- ☛ **We estimate the above kernels in a first stage relying on a subsample of 500 sites - only need 9 kernels**

Shark - implementation (continued)



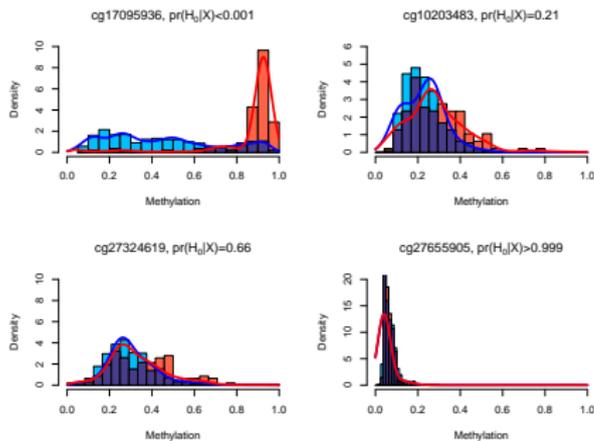
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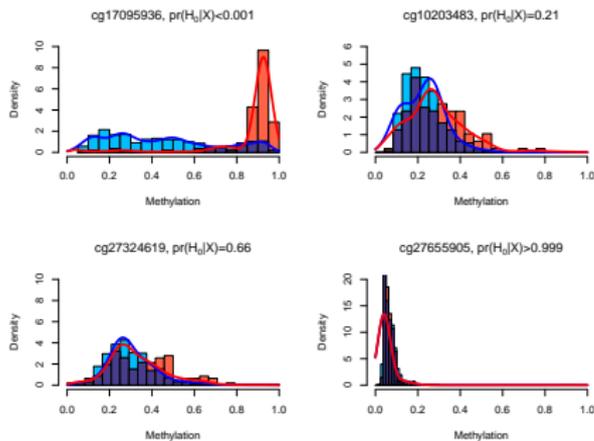
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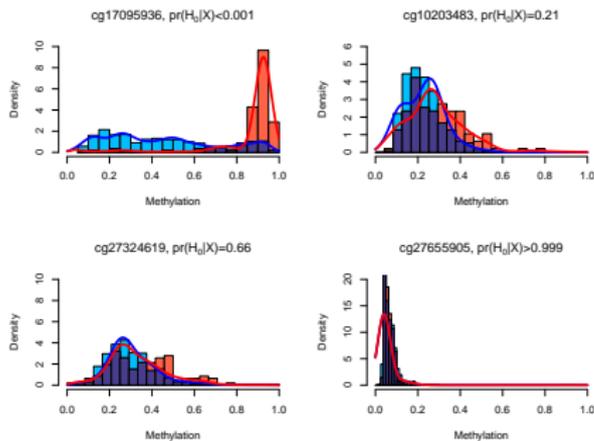
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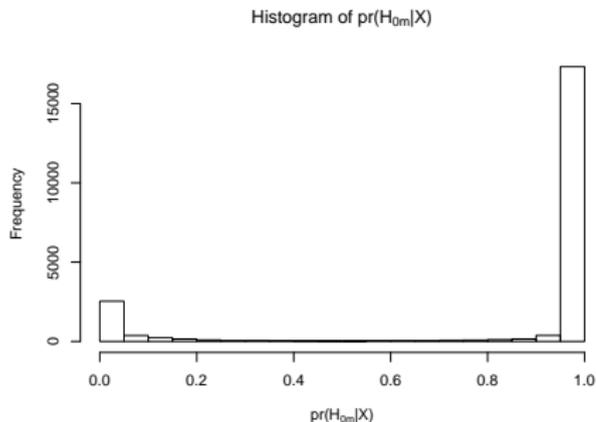
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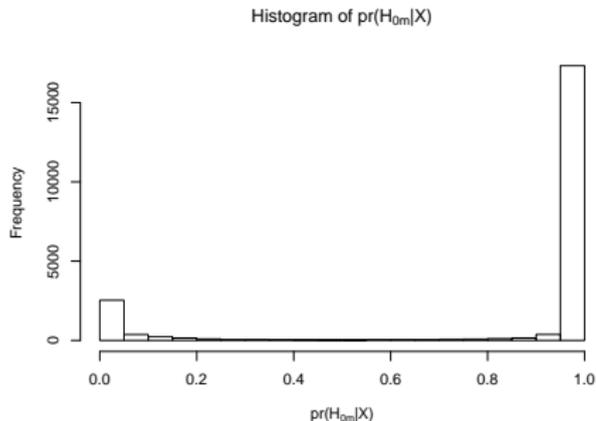
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- ☞ **Theory support, including under misspecification**

Results for Cancer Genome Atlas Data



- ✎ Illustrate using $n = 597$ breast cancer samples & 21,986 CpG sites from TCGA

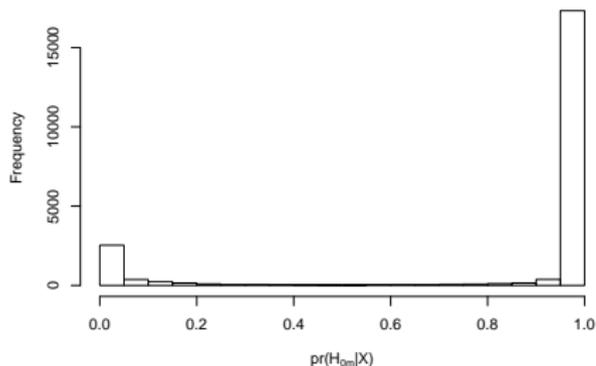
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- ✎ Focus on testing difference between basal-like (112) and not (485) at each site

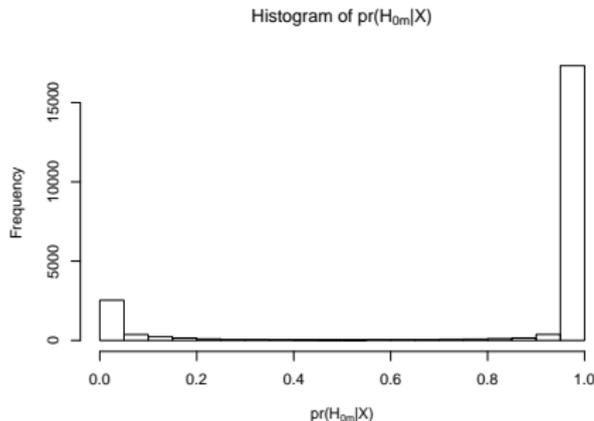
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Histogram of $\text{pr}(H_{0m}|X)$



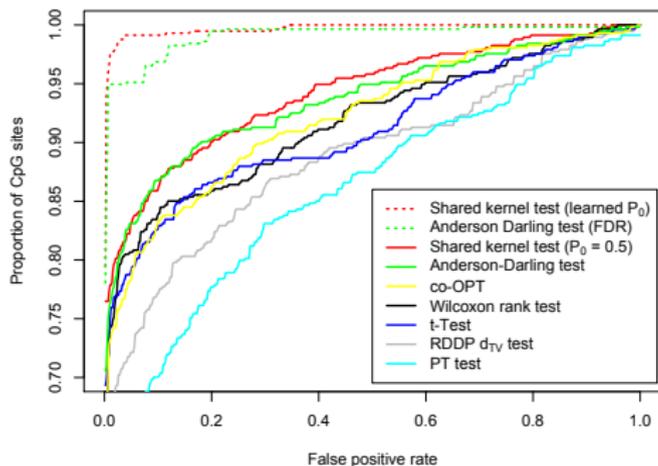
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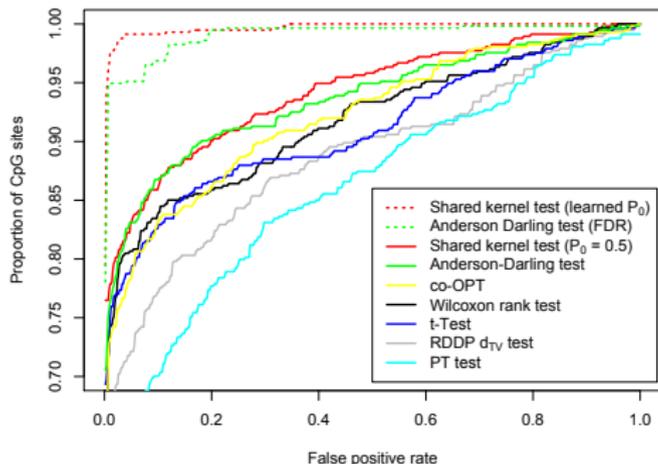
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- ✎ **Distribution of posterior probabilities of H_{0m} shown above**

Discussion & Comparisons



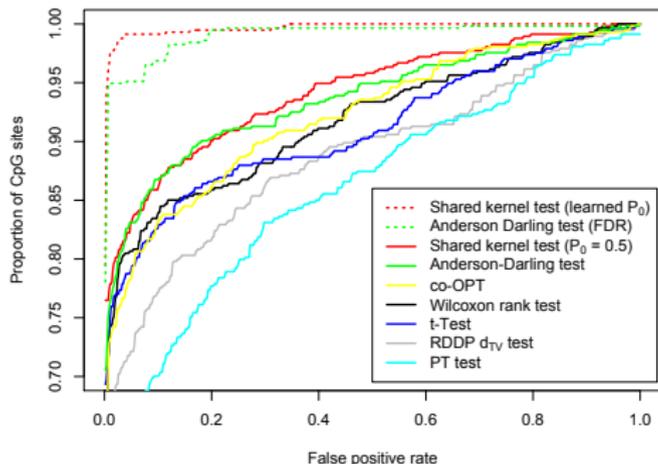
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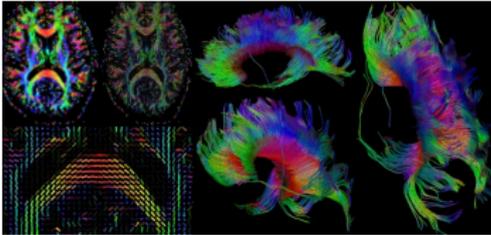
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Discussion & Comparisons



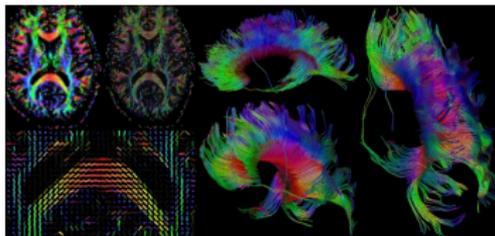
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- ☞ **We compared power of our approach with alternatives**

Shared kernel testing for complex phenotypes



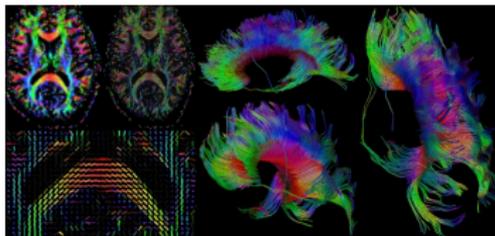
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Shared kernel testing for complex phenotypes



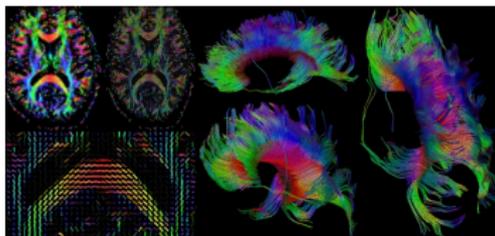
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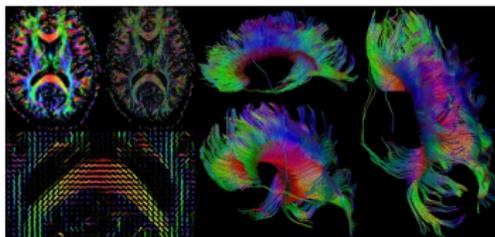
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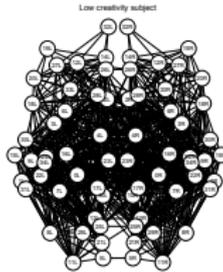
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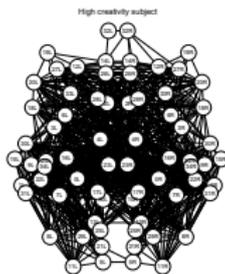
- ☛ Shared kernel approach can be applied to very complex phenotypes
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- ☛ I'll illustrate briefly using brain connectome phenotypes
- ☛ For each individual i , we extract a structural connectome X_i from MRI data
- ☛ Then, $X_{i[u,v]} = 1$ if there 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



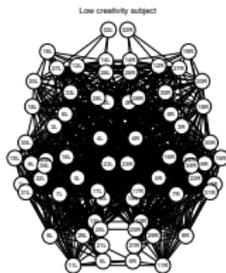
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A nonparametric model of variation in brain networks



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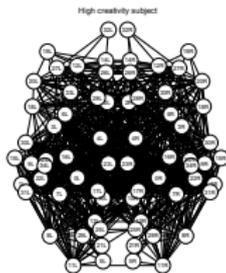
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A nonparametric model of variation in brain networks

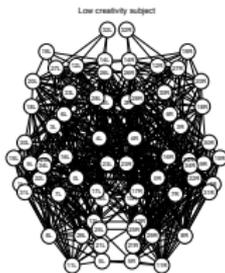


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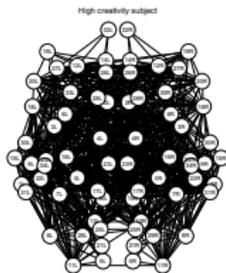


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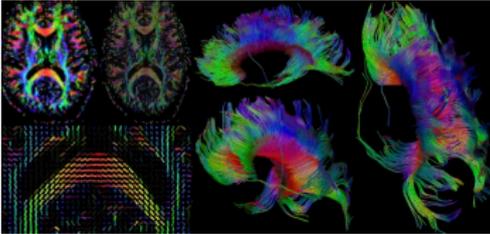


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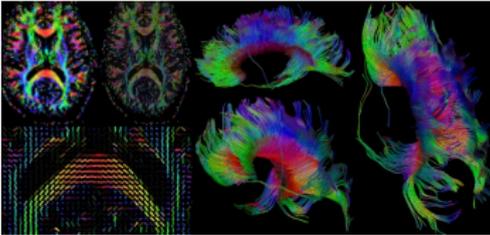
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Bayesian inferences



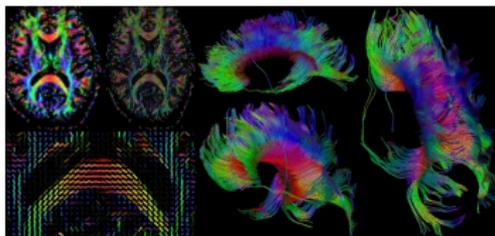
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Bayesian inferences



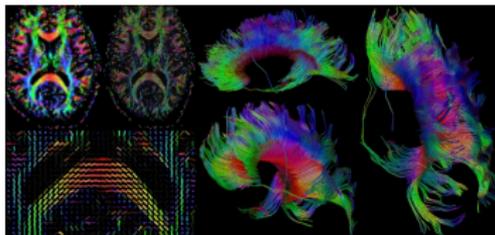
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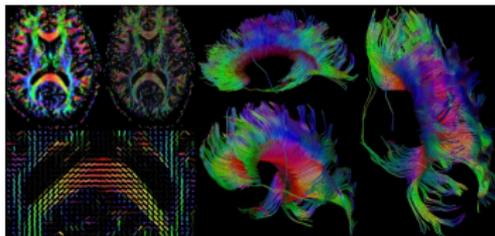
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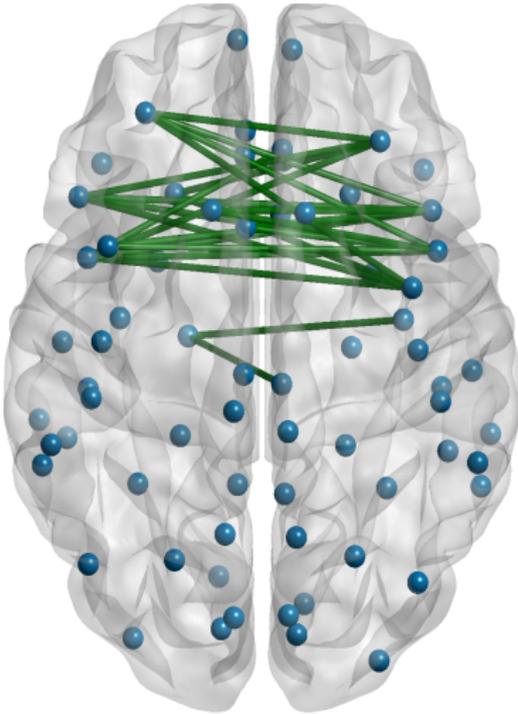
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- ✎ Allows scientific inference of global & local group differences in network structures with traits
- ✎ **Adjusts for multiple testing reducing false positives**

Application to creativity

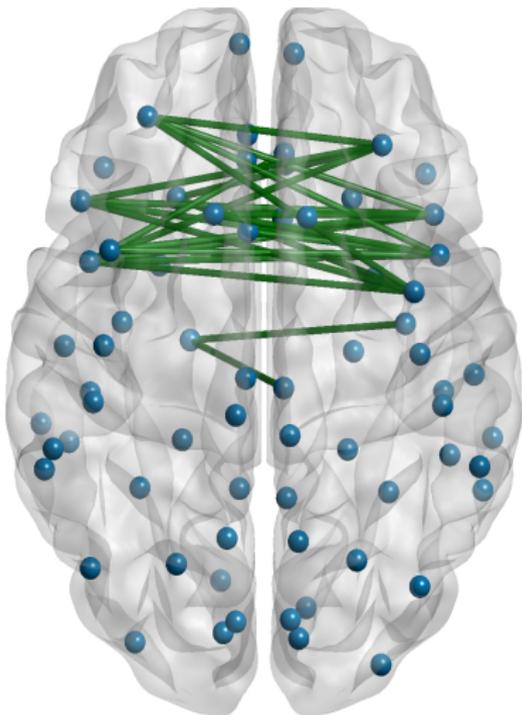
Results from local testing



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

Application to creativity

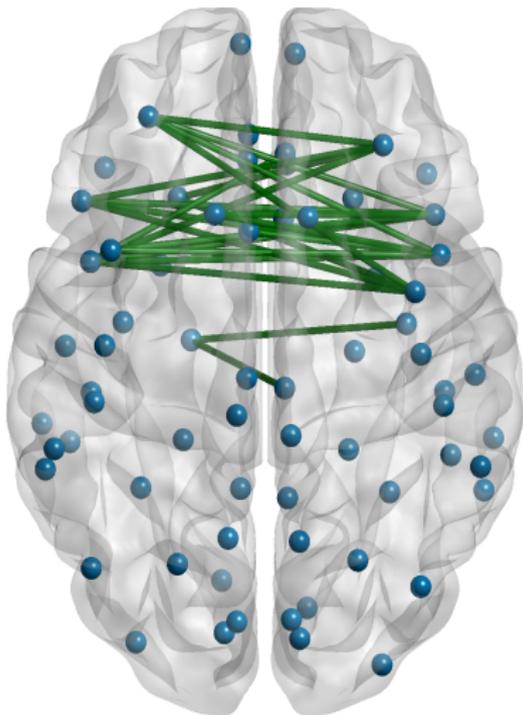
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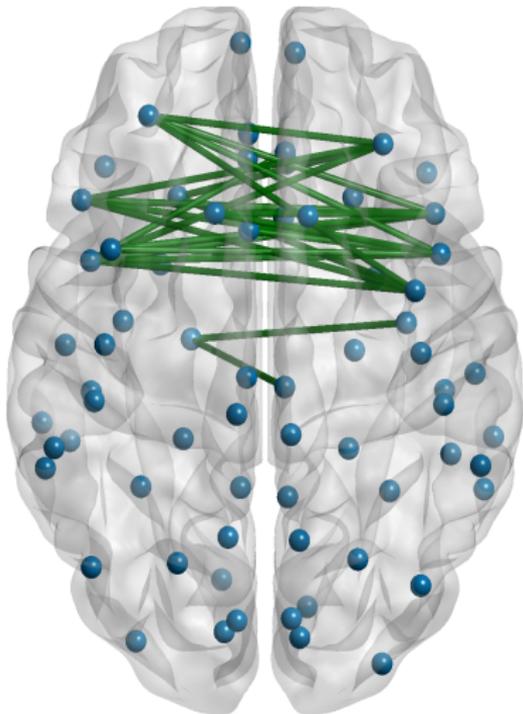
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- Differences in frontal lobe consistent with recent fMRI studies analyzing regional activity in isolation.

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- ✎ **We also want to account for dependence in the many different tests**

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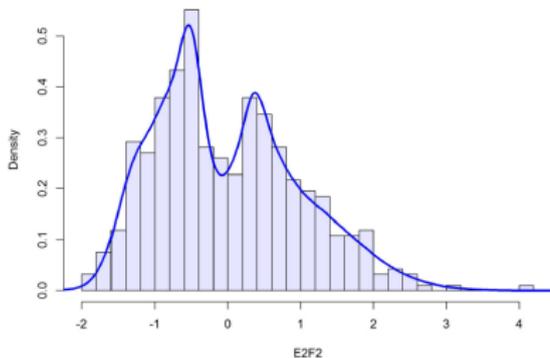
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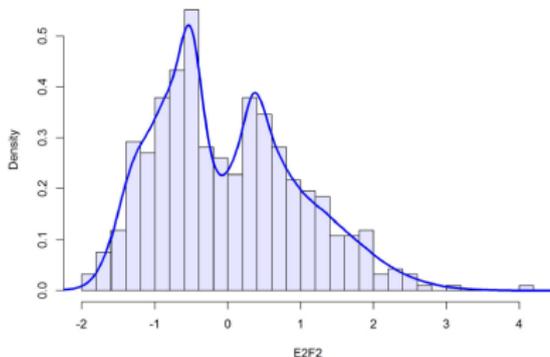
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MOBS - comments



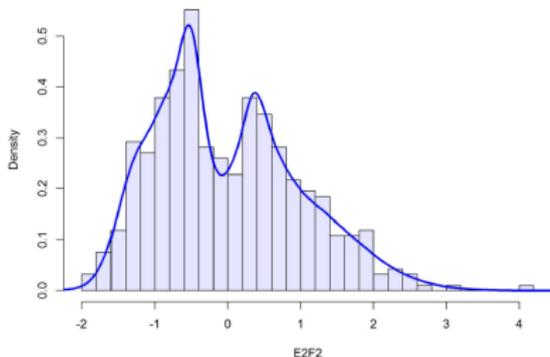
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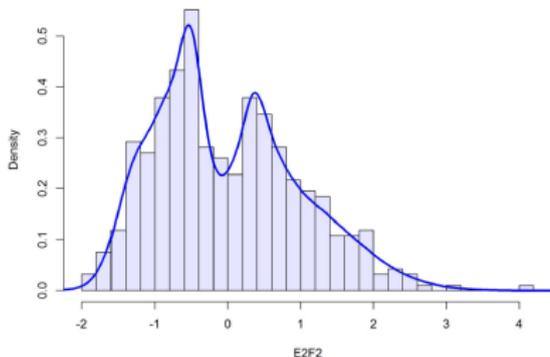
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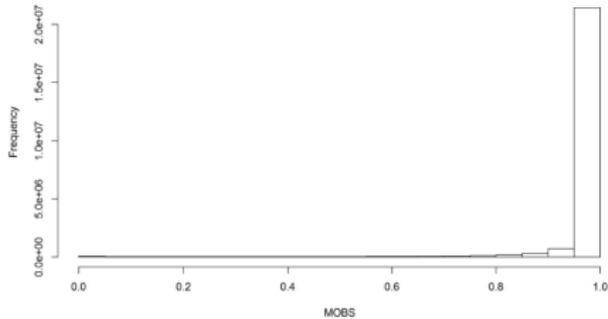
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Application to cis-eQTL data

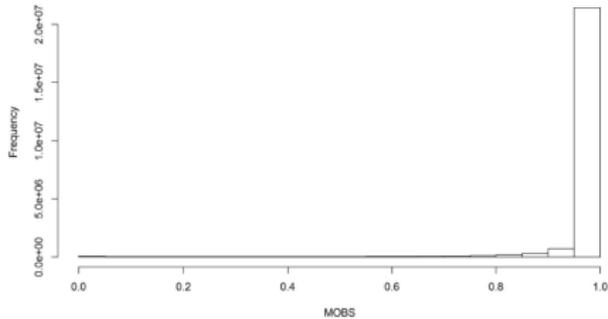
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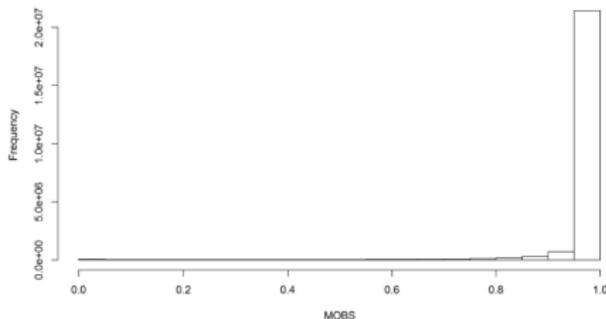
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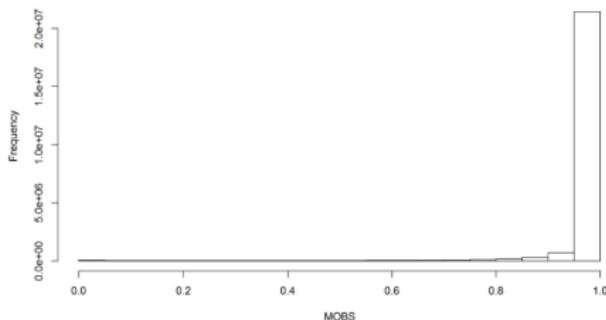
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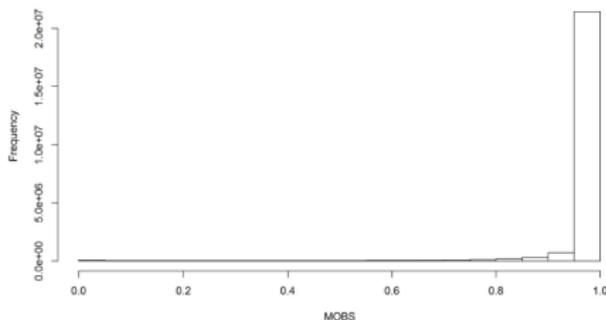
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- ☛ 0.4% of $\text{pr}(H_{0j}) < 0.05$ - picking up differences in distribution other methods miss

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- ✿ **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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- ☛ **Such generalized Bayes methods can have improved computational performance & robustness**