Adventures in sparsity and shrinkage with the normal means model

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The Normal Means problem

$$x_j | \theta_j, s_j \sim N(\theta_j, s_j^2)$$

MLE: $\hat{\theta}_j = x_j$.

Surprise: you can do better than the mle! (Stein, 1956)

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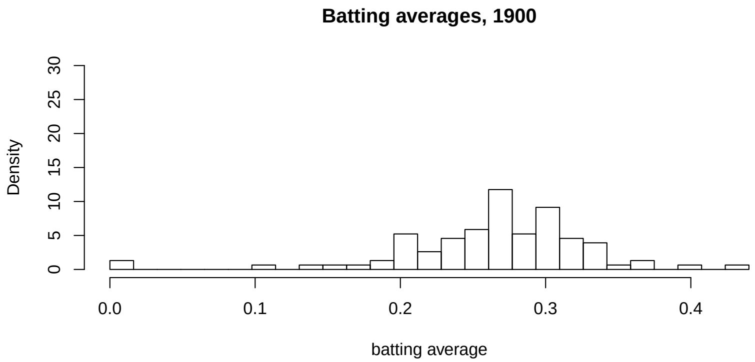

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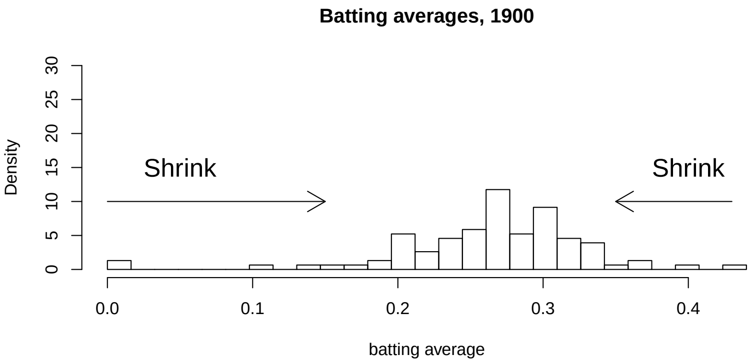

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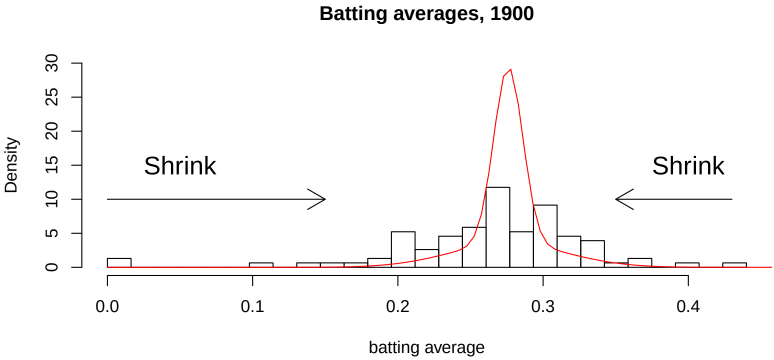

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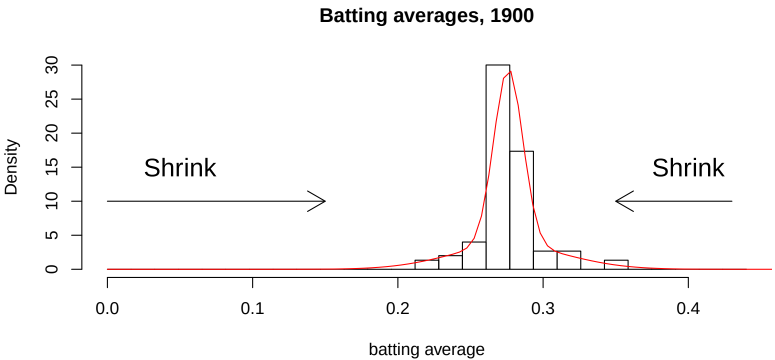

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Empirical Bayes Normal Means (EBNM)

$$x_j|\theta_j, s_j \sim N(\theta_j, s_j^2)$$

$$\theta_j \sim g \in \mathcal{G}$$

Fit this model in two steps:

1. Estimate g by maximizing (marginal) log-likelihood:

$$\widehat{g} = \arg\max \sum_j \log \int p(x_j|\theta_j, s_j) g(d\theta_j)$$

2. Compute posterior distributions $\theta_j \mid \widehat{g}, x_j, s_j$.

“Sparsity-inducing” choices for $\mathcal{G}$

- Point-normal: $\pi_0\delta_0 + (1-\pi_0)N(0,\sigma^2)$.
- Zero-centered scale mixtures of normals (non-parametric; includes point-normal, t, Laplace, horseshoe, ...).

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Simple non-parametric computations

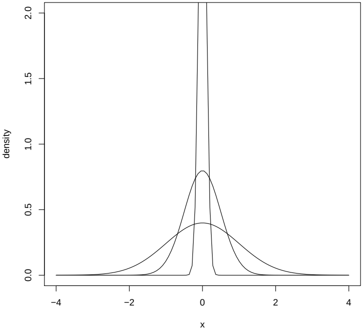
Key idea: approximate non-parametric family by finite mixture with many components:

$$g(\cdot) = \sum_k^K \pi_k N(\cdot; 0, \sigma_k^2)$$

with K big; $\sigma_1, \ldots, \sigma_K$ fixed on a "dense grid".

So estimating g comes down to estimating π.

Illustration: scale mixture of normals



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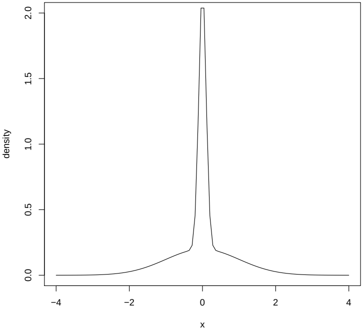


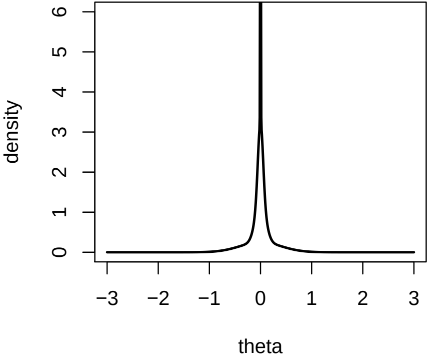
Simple non-parametric computations

This yields simple marginal distribution:

$$p(x_j|\pi) = \sum_k^K \pi_k N(x_j; 0, s_j^2 + \sigma_k^2).$$

And estimating $\pi = (\pi_1, \ldots, \pi_K)$, is a convex optimization problem (Koenker + Mizera, 2015; S. 2017; Kim et al, 2018).

Illustration:Bayesian shrinkage



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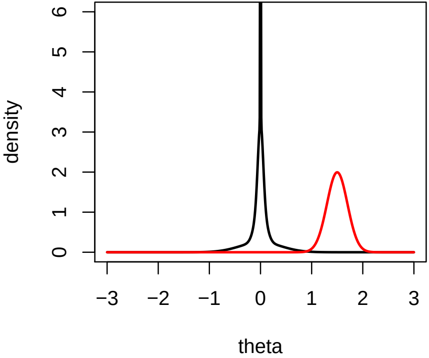

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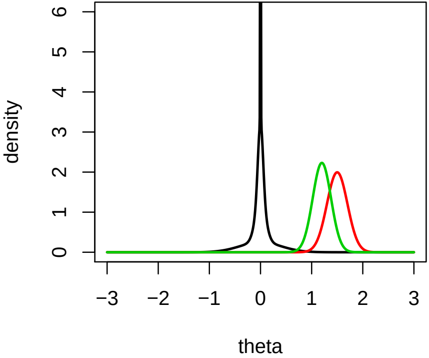

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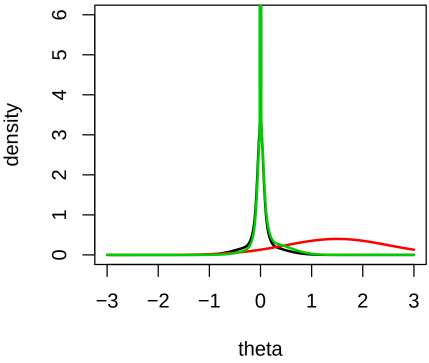

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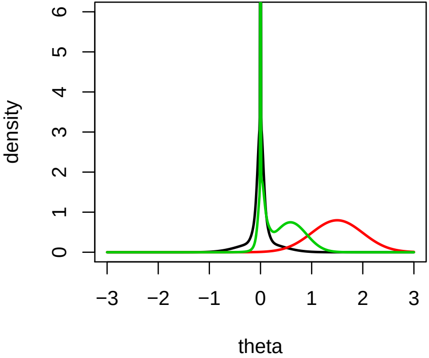


Bayesian shrinkage operators

Shrinkage obviously depends on prior g (and standard error s_j).

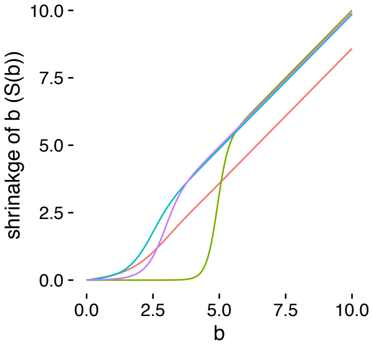
One way to summarize shrinkage behavior is to focus on how posterior mean changes with x:

$$S_{g,s}(x) := E(\theta_j | x_j = x, g, s_j = s)$$

Call this the "shrinkage operator" for prior g.

Bayesian shrinkage operators

Example shrinkage operators for different priors (scale mixtures of normals, $s = 1$):



Shrinkage operators via penalized likelihood

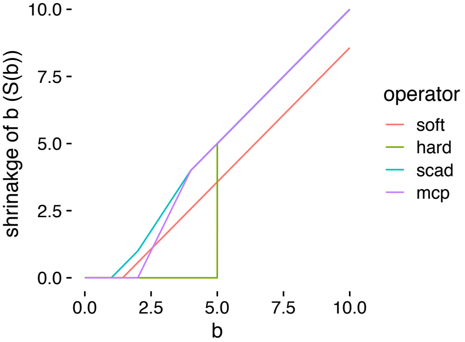
Another way to induce shrinkage/sparsity is penalized log-likelihood:

$$\hat{\theta}_j = S_{h,\lambda}(x) := \arg\min_{\theta} \left[0.5(x-\theta)^2 + \lambda h(\theta)\right]$$

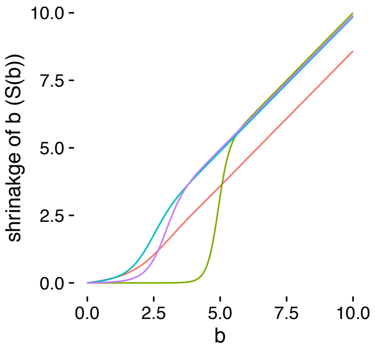
where h a penalty function, and λ a tuning parameter.

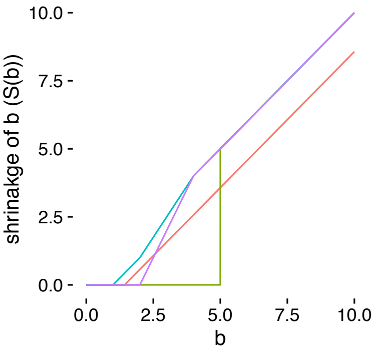
[Can think of these as posterior mode under some prior, but I don't recommend it!]

Penalty-based shrinkage operators



Bayesian vs Penalty-based shrinkage operators





Key features of EB shrinkage

1. Shrinkage determined by g, which is estimated by maximum likelihood, rather than CV.
2. Very flexible: can mimic a range of penalty functions.
3. Posterior distribution $\theta_j \mid \widehat{g}, x_j, s_j$ gives not only shrunken point estimates but also "shrunken" interval estimates.

...despite this, until recently little attention paid to EB shrinkage in practical applications.

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Example Applications

- Multiple testing
- Linear Regression
- Matrix factorization

Multiple Testing

Typical set-up (e.g. Benjamini and Hochberg, 1995):

- Large number of tests $j = 1, \ldots, n$.
- Test j yields p value p_j.
- Reject all tests with $p_j < \gamma$ with $\gamma(p)$ chosen to control FDR.

Multiple Testing via EBNM

In many applications p values are derived from effect estimates, $\hat{\beta}_j$, and standard errors s_j, satisfying:

$$\hat{\beta}_j \sim N(\beta_j, s_j^2).$$

Aim: identify β_j that are different from zero.

Ideally suited to EBNM!

Multiple Testing via EBNM

$$\hat{\beta}_j | \beta_j \sim N(\beta_j, s_j^2)$$

$$\beta_j \sim g() \in \mathcal{G}$$

Estimate $\hat{g}$ by maximum likelihood; compute posterior 90% interval for each β_j; reject if interval does not contain 0.

Details: S. (2017); see also Thomas (1985), Efron (200x).

EBNM vs BH for multiple testing

- EBNM slightly more powerful.
- BH more robust to correlated tests (but see Sun + S. (2019)).
- EBNM provides shrinkage interval estimates! (e.g. address winner's curse)

But real benefit of EBNM maybe comes in multivariate extensions...

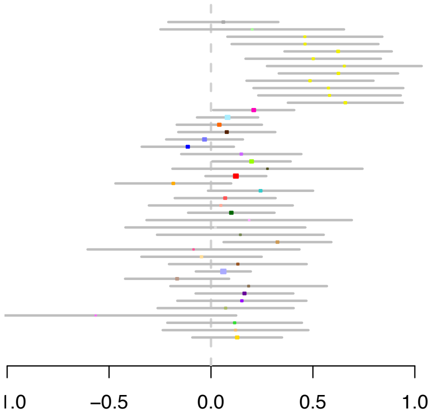
Multivariate multiple testing (Urbut et al, 2018)

$$\hat{\boldsymbol{\beta}}_j | \boldsymbol{\beta}_j \sim N_r(\boldsymbol{\beta}_j, V_j)$$

$$\boldsymbol{\beta}_j \sim g(\cdot) = \sum_k \pi_k N_r(0, \Sigma_k)$$

Multivariate multiple testing (Urbut et al, 2018)

Eg: eQTL effect sizes across 44 tissues (GTEx Consortium, 2017).



Multivariate multiple testing

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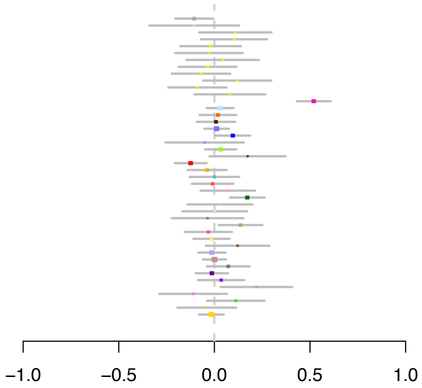
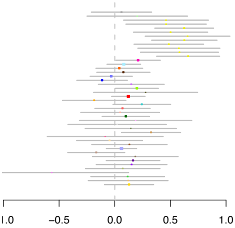
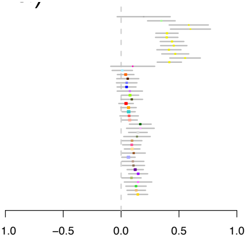


Multivariate multiple testing

a) Data



b) Posterior



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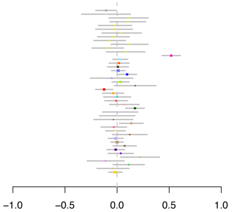

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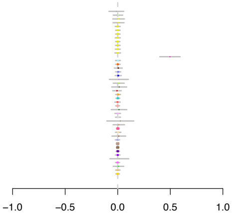

Linear regression

$$\mathbf{y}_{n\times 1} = X_{n\times p}\mathbf{b}_{p\times 1} + \mathbf{e}_{n\times 1}$$

$$\mathbf{e} \sim N_n(0, \sigma^2 I_n)$$

$$b_1, \ldots, b_p \sim g() \in \mathcal{G}$$

Challenge: how to apply EBNM ideas here?

An analogy: Penalized regression

Penalized linear regression solves:

$$\hat{\mathbf{b}} = \arg\min_{\mathbf{b}} 0.5||\mathbf{y} - X\mathbf{b}||_2^2 + \lambda \sum_j h(b_j)$$

E.g. $h(b) = b^2$ gives ridge regression; $h(b) = |b|$ gives lasso.

Coordinate Ascent Iterative Shrinkage Algorithm (CAISA)

For each coordinate j, update b_j as follows:

- Compute residuals $\mathbf{r}_j := \mathbf{y} - X_{-j}\mathbf{b}_{-j}$
- Compute $\hat{b}_j = (\mathbf{x}_j^T \mathbf{x}_j)^{-1} \mathbf{x}_j^T \mathbf{r}_j$
- Shrink: $b_j := S_{h,\lambda}(\hat{b}_j)$

where S is a shrinkage operator for h, λ:

$$S_{h,\lambda}(b) := \arg\min_a (b-a)^2 + \lambda h(a).$$

g-CAISA:

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- Compute $s_j := (\mathbf{x}_j^T \mathbf{x}_j)^{-1} \sigma^2$
- Shrink: $b_j := S_{g,s_j}(\hat{b}_j)$

where S is the posterior mean shrinkage operator determined by prior g.

What is this doing?

Define:

$$F(q) := -KL(q \to p(b|X, \mathbf{y}, g, \sigma^2))$$

$$\mathcal{Q} := \{q : q(\mathbf{b}) = \prod_{j=1}^{p} q_j(b_j)\}$$

Proposition (Kim et al, in prep): The g-CAISA algorithm is a coordinate ascent algorithm for maximizing $F(q)$ (i.e. minimizing KL) over $q \in \mathcal{Q}$, with $\mathbf{b}$ the expectation of q.

Estimating g?

Recall algorithm:

- Compute residuals $\mathbf{r}_j := \mathbf{y} - X_{-j}\mathbf{b}_{-j}$
- **Compute** $\hat{b}_j := (\mathbf{x}_j^T \mathbf{x}_j)^{-1} \mathbf{x}_j^T \mathbf{r}_j$
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Idea: after computing $\hat{b}_j, s_j$ for $j = 1, \ldots, p$, apply EBNM to estimate g.

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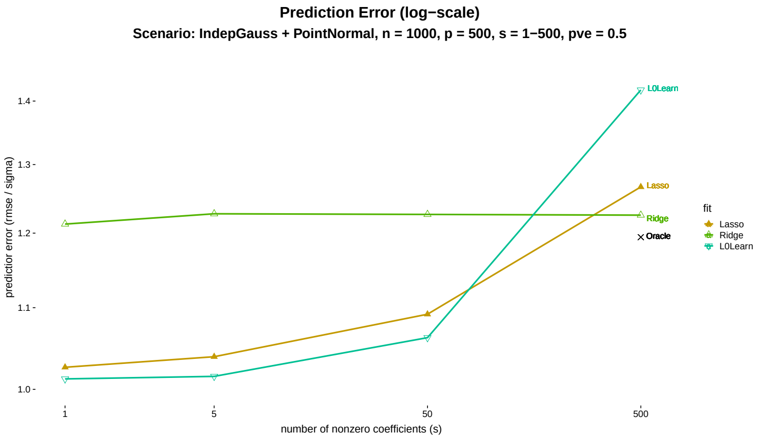
Simulation Results



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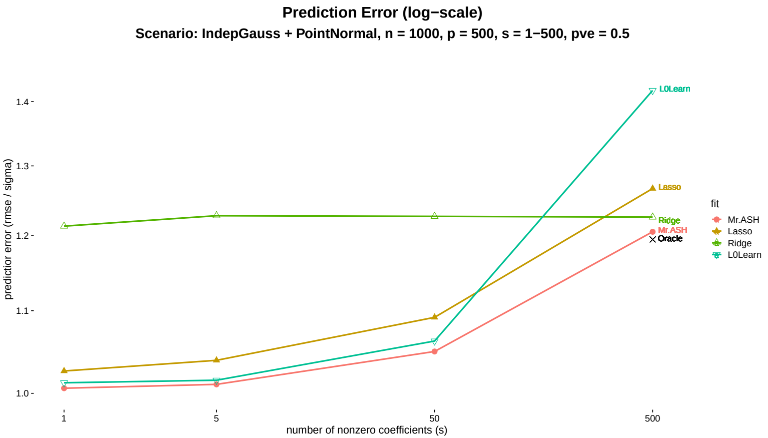
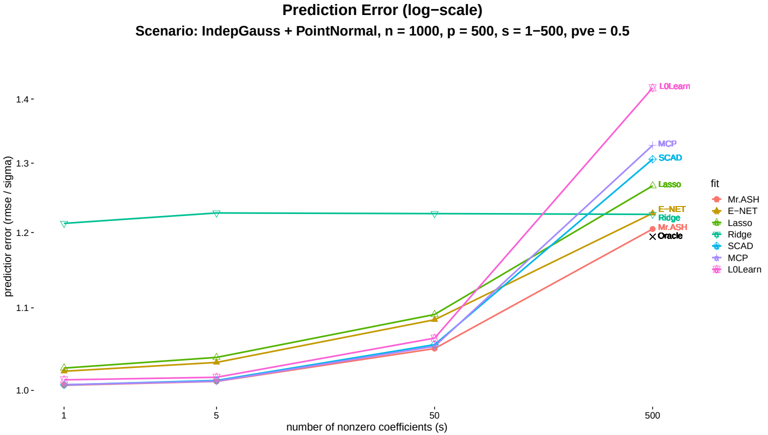


Simulation Results - more penalties



Matrix factorization

$$Y_{n \times p} = L_{n \times K} F^T_{K \times p} + E_{n \times p}$$

Common Assumption: F and/or L are sparse.

But how sparse?

Empirical Bayes Matrix Factorization: rank $K = 1$

$$Y = lf^T + E$$

$$l_1, \ldots, l_n \sim g^l(\cdot) \in \mathcal{G}$$
$$f_1, \ldots, f_p \sim g^f(\cdot) \in \mathcal{G}$$

Algorithm, in outline, iterates:

- Given f, estimate g^l, l by solving EBNM problem.
- Given l, estimate g^f, f by solving EBNM problem.

Optimizes a variational approximation to the posterior.

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Algorithm, in outline, iterates:

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Optimizes a variational approximation to the posterior.

Empirical Bayes Matrix Factorization: rank $K > 1$

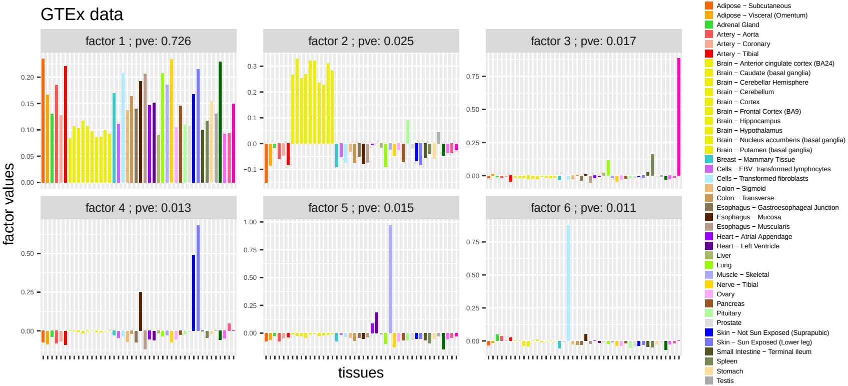
$$Y = \sum_{k=1}^{K} l_k f_k^T + E$$

$$l_{k1}, \ldots, l_{kn} \sim g_k^l(\cdot) \in \mathcal{G}$$
$$f_{k1}, \ldots, f_{kp} \sim g_k^f(\cdot) \in \mathcal{G}$$

Iterative solution, updating $k = 1, \ldots, K$ using rank 1.

Details: Wang + S. (2018)

GTEx data: first 6 factors



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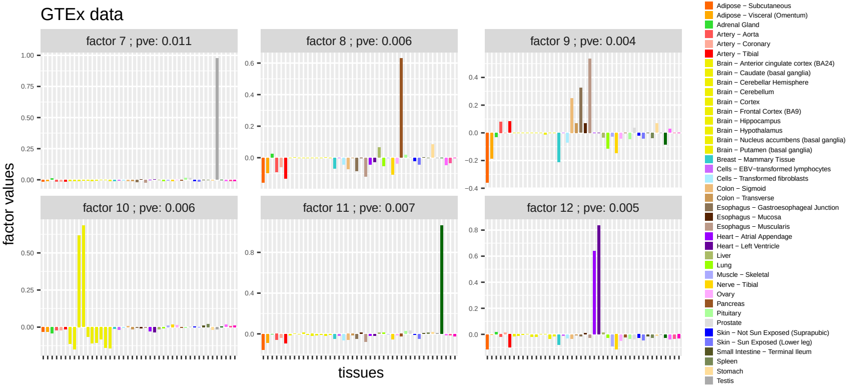
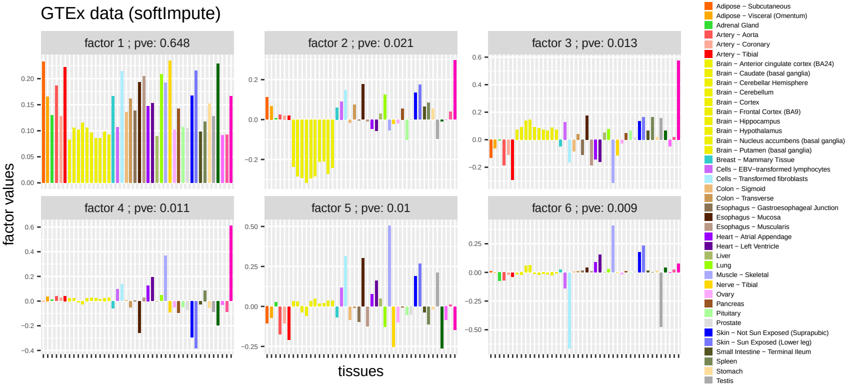


Comparison: softImpute (nuclear norm penalty)



Summary

EBNM provides a flexible and convenient way to induce shrinkage and sparsity in a range of applications.

More Details

http://stephenslab.uchicago.edu/publications.html

- Multiple Testing: Efron (200x); S. (2017); Urbut et al (2017), Gerard + S. (2018).
- Linear Regression: Wang (2018); Kim et al (in prep).
- Matrix factorization: Wang and S. (2018).
- Wavelets: Johnstone + Silverman (2004); Xing, Carbonetto + S. (2017).
- Correlation: Dey and S. (2018).