I-priors in Bayesian Variable Selection: From Reproducing Kernel Hilbert Spaces to Hamiltonian Monte Carlo

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Social Statistics Meeting

follow along at: **https://haziqjamil.github.io/**

Outline

The I-prior Bayesian Variable Selection model

- For centred responses y_i and standardised covariates $x_{i1}, \dots, x_{ip}$,

$$\begin{gathered} y_i = \gamma_1 \beta_1 x_{i1} + \cdots + \gamma_p \beta_p x_{ip} + \epsilon_i \\ \epsilon_i \sim \mathrm{N}(0, \psi^{-1}) \\ i = 1, \dots, n \\ \\ \underline{\text{Priors}} \\ \boldsymbol{\beta} \sim \mathrm{N}(\mathbf{0}, \psi \boldsymbol{\Lambda} \mathbf{X}^\top \mathbf{X} \boldsymbol{\Lambda}), \ \text{where } \boldsymbol{\Lambda} = \mathrm{diag}[\lambda_1, \dots, \lambda_p] \\ \gamma_j \sim \mathrm{Bern}(p_j), \ j = 1, \dots, p \\ \psi, \lambda_1^{-2}, \dots, \lambda_p^{-2} \sim \Gamma(c, d) \end{gathered} \tag{1}$$

- Use MCMC methods to sample from posterior using software such as JAGS. Interested in two things:
  - Posterior model probabilities $\mathrm{P}[\boldsymbol{\gamma} = \boldsymbol{\gamma}' | \mathbf{y}]$ for model $\boldsymbol{\gamma}'$.
  - Posterior inclusion probabilities $\mathrm{P}[\gamma_j = 1 | \mathbf{y}]$ for variable X_j.

Why Bayesian Variable Selection?

Some criticisms

- The end-game of model selection is often prediction. If so, better methods exist e.g. Lasso
- Why not just put a reasonable prior?
- Unreliable Gibbs sampler - likely to get stuck in multiple modes.

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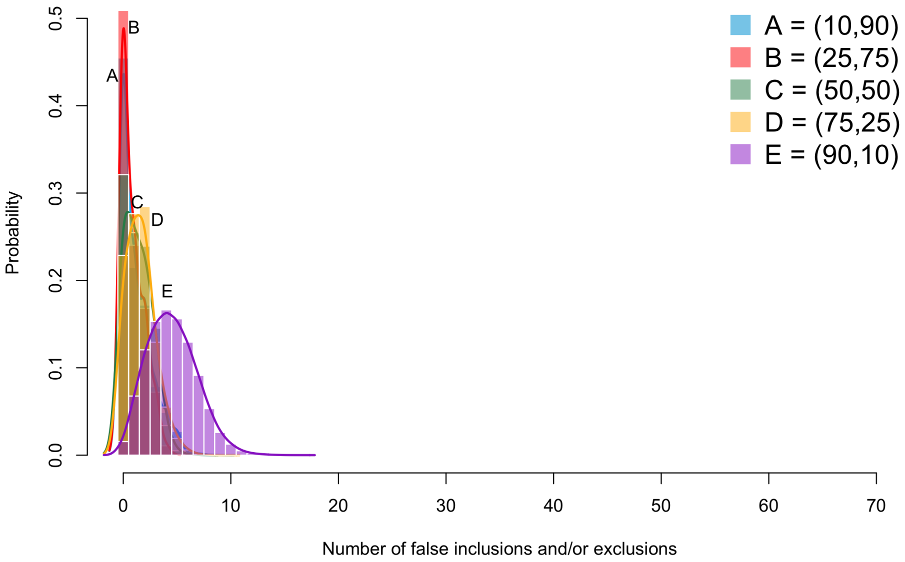
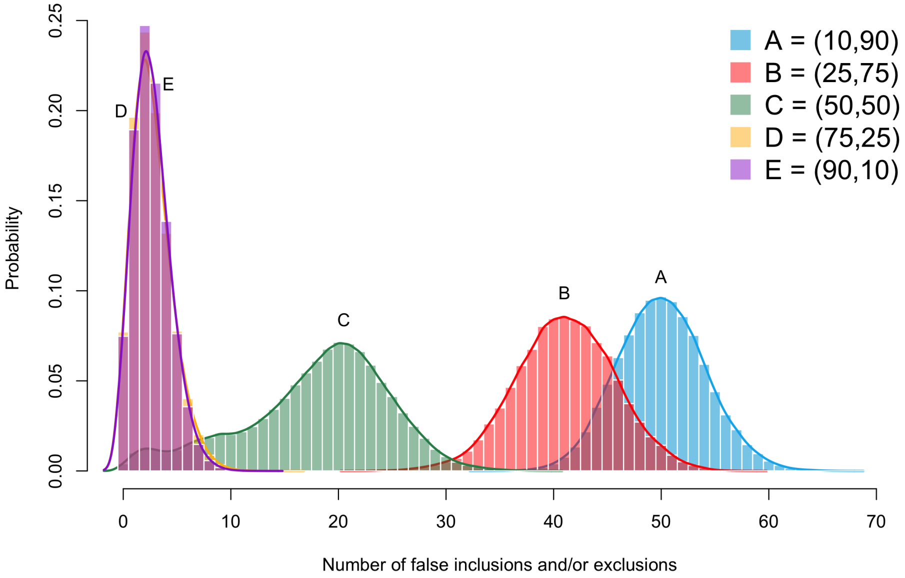
But actually,

- Sometimes there is a need to know what is the most plausible, interpretable, and parsimonious model.
- Valid applications in social sciences, but perhaps not the $p > n$ cases.
- Gibbs sampler not too terrible.
- For as many critics to this "combinatorial approach", there are equally as many proponents.
- Prediction through Bayesian model averaging.

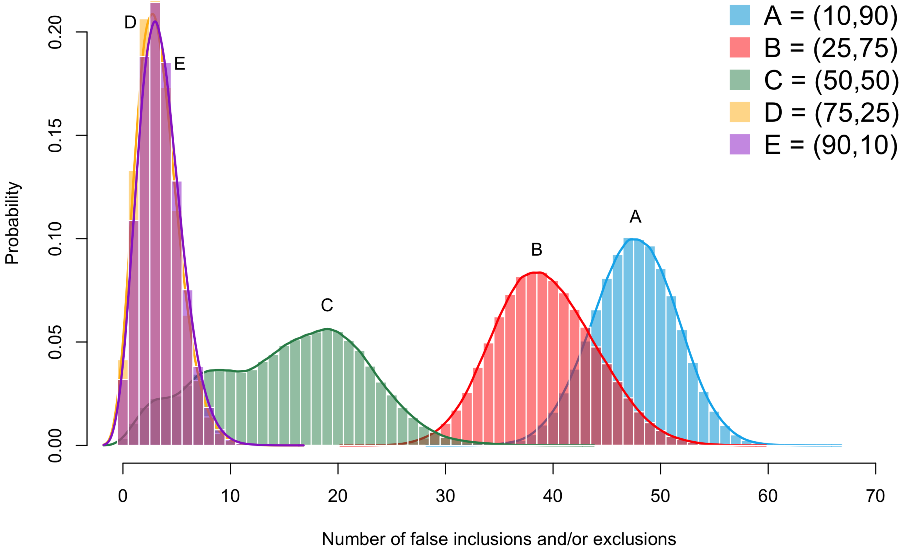
Simulation results are good...



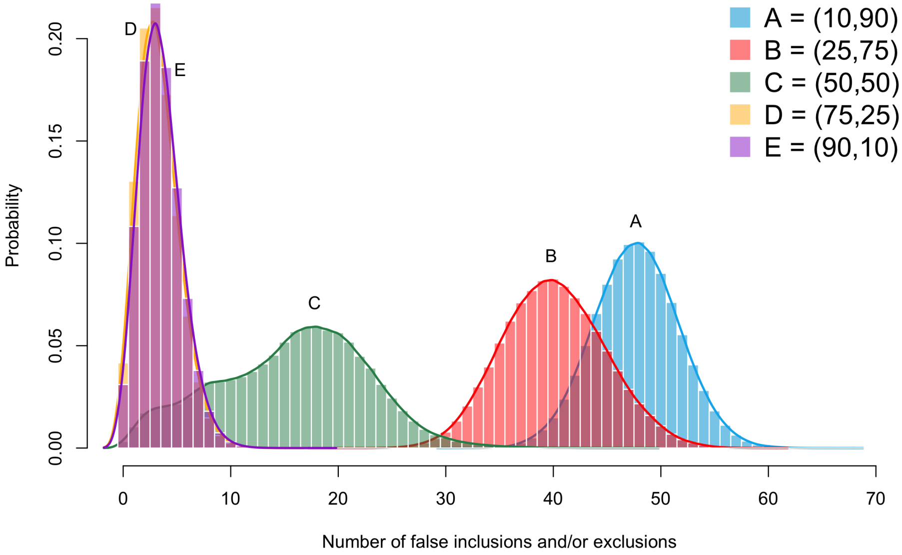
...in comparison to: SSVS (George & McCulloch, 1993)



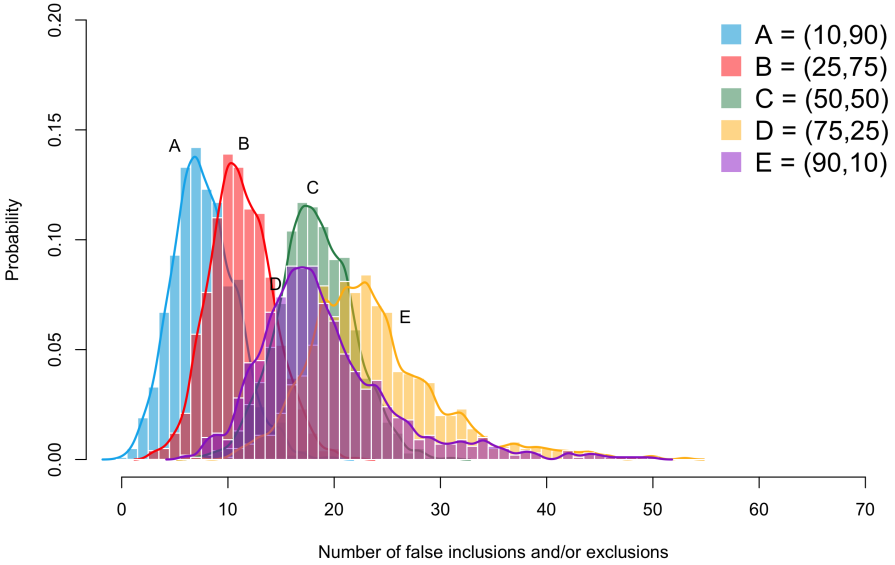
...in comparison to: KM (Kuo & Mallick, 1998)



...in comparison to: GVS (Dellaportas et. al., 2011)



...in comparison to: Lasso (Tibshirani, 1994)



...and so are some real world applications

1. **Modelling aerobic fitness through some exercise data** ($n = 30$, $p = 6$) [Kuo and Mallick, 1998]
   - Agreed with forward selection and backward elimination procedure except in the `Age` variable.
   - `Age` negatively correlated with `MaxPulse`.

2. **Effects of air pollution on mortality rate** ($n = 60$, $p = 15$) [McDonald and Schwing, 1973]
   - Which of `HC`, `NOx`, and/or `SO2` affects mortality rate in U.S. metropolitan areas?
   - Agreed with "ridge trace analysis" in identifying `SO2`.

3. **Factors affecting ozone depletion** ($n = 178$, $p = 12, 90$) [Casella and Moreno, 2006]
   - Model obtained had smaller out-of-sample RMSE.
   - Selection of squared and two-way interaction terms to improve RMSE without overcomplicating the model.

Introduction

- For $i = 1, \dots, n$, consider the regression model

$$\begin{gathered} y_i = \alpha + f(\mathbf{x}_i) + \epsilon_i \\ (\epsilon_1, \dots, \epsilon_n) \sim \mathrm{N}(\mathbf{0}, \mathbf{\Psi}^{-1}) \end{gathered} \tag{2}$$

where $f \in \mathcal{F}$, $y_i \in \mathbb{R}$, and $\mathbf{x}_i = (x_{i1}, \dots, x_{ip}) \in \mathcal{X}$.

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- Definition **(I-priors)**

  For the regression model above, let $\mathcal{F}$ be a reproducing kernel Hilbert space (RKHS) with kernel $h_{\boldsymbol{\lambda}} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. Then, assuming it exists, the Fisher information for $I[f]$ for the function f is given by

$$I[f(\mathbf{x}_i), f(\mathbf{x}_i')] = \sum_{k=1}^n \sum_{l=1}^n \psi_{kl} h_{\boldsymbol{\lambda}}(\mathbf{x}_i, \mathbf{x}_k) h_{\boldsymbol{\lambda}}(\mathbf{x}_i', \mathbf{x}_l).$$

  Let π be a Gaussian distribution on the random vector f with mean f_0 and covariance kernel $I[f]$. Then π is called an I-prior for f.

Function spaces and kernels

- There is a bijection between the set of all positive-definite functions (reproducing kernels) $h : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ and the set of all RKHS.

$\mathcal{X} = \{x_i\}$	**Effect**	**Vector space** $\mathcal{F}$	**Kernel** $h(x_i, x_k)$
Real	"Straight line" functions	Canonical	$x_i x_k$
Real	"Curvy" functions (smoothing)	Fractional Brownian Motion (FBM)	$\lvert x_i\rvert^{2\gamma} + \lvert x_k\rvert^{2\gamma} - \lvert x_i - x_k\rvert^{2\gamma}$ with $\gamma \in (0,1)$
Nominal	Grouping	Pearson	$\frac{\mathbb{1}[x_i = x_k]}{p_i} - 1$ where $p_i = \mathrm{P}[X = x_i]$

The w I-prior model

- The I-prior for f has the random-effect representation

$$f(\mathbf{x}_i) = \alpha + f_0(\mathbf{x}_i) + \sum_{k=1}^{n} h_{\boldsymbol{\lambda}}(\mathbf{x}_i, \mathbf{x}_k) w_k$$

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- Parameters of interest are $\boldsymbol{\theta} = (\alpha, \lambda_1, \dots, \lambda_p, \psi)$.

Maximum likelihood

- The marginal distribution of $\mathbf{y}$ is normal with mean and variance

$$\mathrm{E}[\mathbf{y}] = \boldsymbol{\alpha}$$
$$\mathrm{Var}[\mathbf{y}] = \psi \mathbf{H}_{\boldsymbol{\lambda}}^2 + \psi^{-1}\mathbf{I}_n =: \mathbf{V}_y$$

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and thus, the marginal log-likelihood is given by

$$l(\boldsymbol{\theta}) = -\frac{n}{2}\log(2\pi) - \frac{1}{2}\log|\mathbf{V}_y| - \frac{1}{2}(\mathbf{y}-\boldsymbol{\alpha})^\top \mathbf{V}_y^{-1}(\mathbf{y}-\boldsymbol{\alpha}).$$

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- *Problem: Convergence is difficult when there are a lot of scale parameters.*

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  - $\mathbf{w} \sim \mathrm{N}(\mathbf{0}, \psi \mathbf{I}_n)$
  - $\begin{pmatrix} \mathbf{y} \\ \mathbf{w} \end{pmatrix} \sim \mathrm{N}\left(\begin{pmatrix} \boldsymbol{\alpha} \\ \mathbf{0} \end{pmatrix}, \begin{pmatrix} \mathbf{V}_y & \psi \mathbf{H}_{\boldsymbol{\lambda}} \\ \psi \mathbf{H}_{\boldsymbol{\lambda}} & \psi \mathbf{I}_n \end{pmatrix} \right)$
  - $\mathbf{w} | \mathbf{y} \sim \mathrm{N}\left(\psi \mathbf{H}_{\boldsymbol{\lambda}} \mathbf{V}_y^{-1} (\mathbf{y} - \boldsymbol{\alpha}), \mathbf{V}_y^{-1} \right)$

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  - $\mathbf{w}|\mathbf{y} \sim \mathrm{N}\left(\psi \mathbf{H}_{\boldsymbol{\lambda}} \mathbf{V}_y^{-1}(\mathbf{y} - \boldsymbol{\alpha}), \mathbf{V}_y^{-1} \right)$
- For $t = 0, 1, \ldots,$ do:
  - E-step: Calculate $Q(\boldsymbol{\lambda}, \psi) = \mathrm{E}_{\mathbf{w}} \left[\log f(\mathbf{y}, \mathbf{w}; \boldsymbol{\theta}) | \mathbf{y}; \boldsymbol{\lambda}^{(t)}, \psi^{(t)}, \hat{\alpha} \right]$.
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- *Problem: May be very slow to converge.*

The R/iprior package

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- Example: Look at how students' mathematics achievement varies across different high schools (High School & Beyond dataset).

```
str(hsbsmall)

## 'data.frame': 661 obs. of  3 variables:
##  $ mathach : num  16.663 -2.155 0.085 18.804 2.409 ...
##  $ ses     : num  0.322 0.212 0.682 -0.148 -0.468 0.842 ..
##  $ schoolid: Factor w/ 16 levels "1374","1433",..: 1 1 1..
```

The R/iprior package

- Fit a straight line regressing `mathach` against `ses`.

```
system.time(
  mod <- iprior(mathach ~ ses, data = hsbsmall)
)

## Iteration 0:    Log-likelihood = -19755.905 .......
## Iteration 100:  Log-likelihood = -2169.8515 ........
## Iteration 200:  Log-likelihood = -2169.8481 ....
## Iteration 258:  Log-likelihood = -2169.8481
## EM complete.
##    user  system elapsed
##  90.677   1.946  92.752
```

The R/iprior package

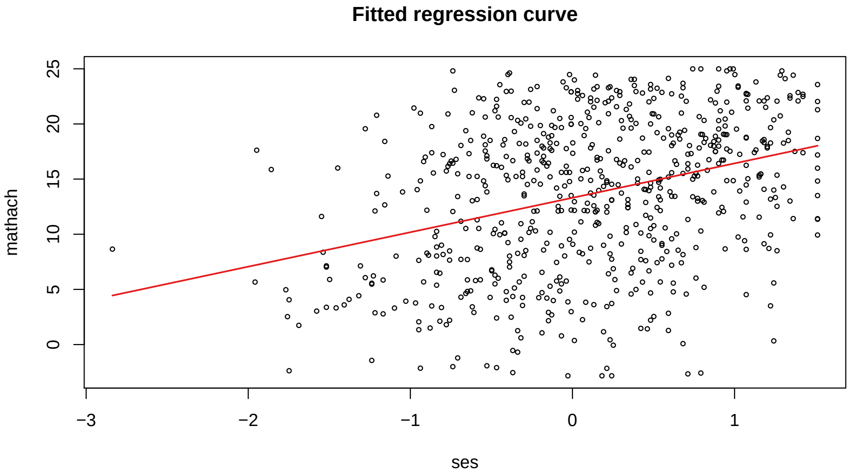
- Obtain the parameter estimates. Can also do `summary(mod)`.

```
print(mod)

##
## Call:
## iprior(formula = mathach ~ ses, data = hsbsmall)
##
## RKHS used: Canonical, with a single scale parameter.
##
##
## Parameter estimates:
## (Intercept)      lambda         psi
## 13.68325416  1.06084515  0.02421674
```

The R/iprior package

```r
plot(mod, plots = "fitted")
```



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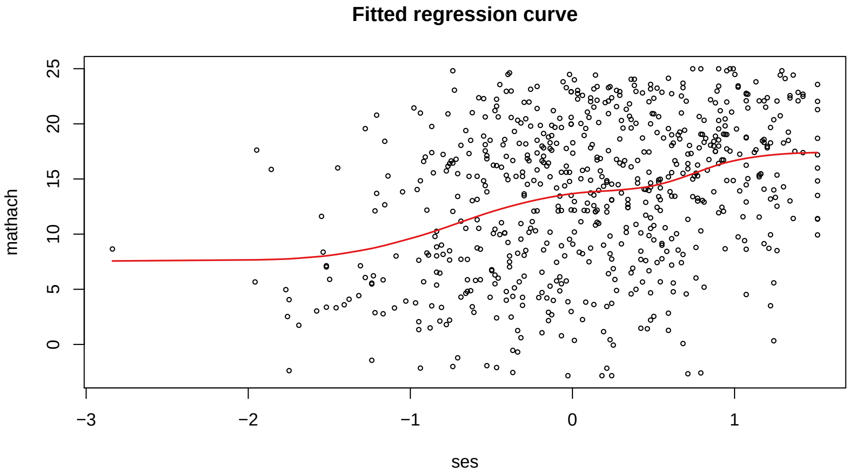
```
plot(
  iprior(mathach ~ ses, hsbsmall, model = list(kernel = "FBM"))
)
```



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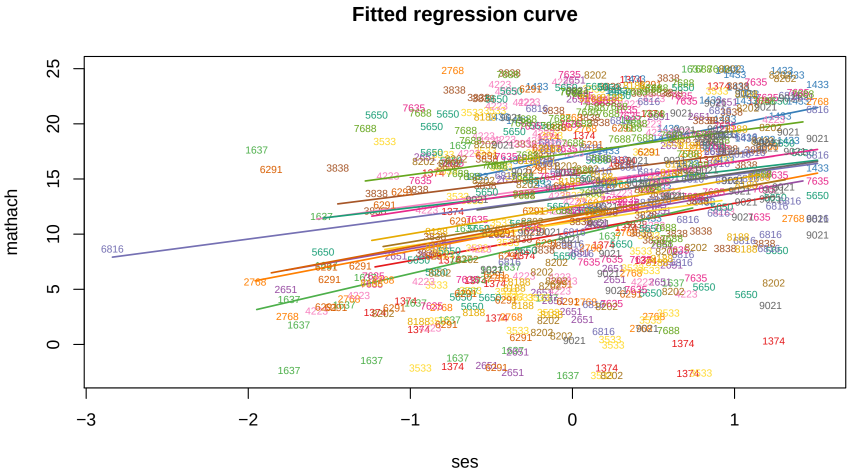
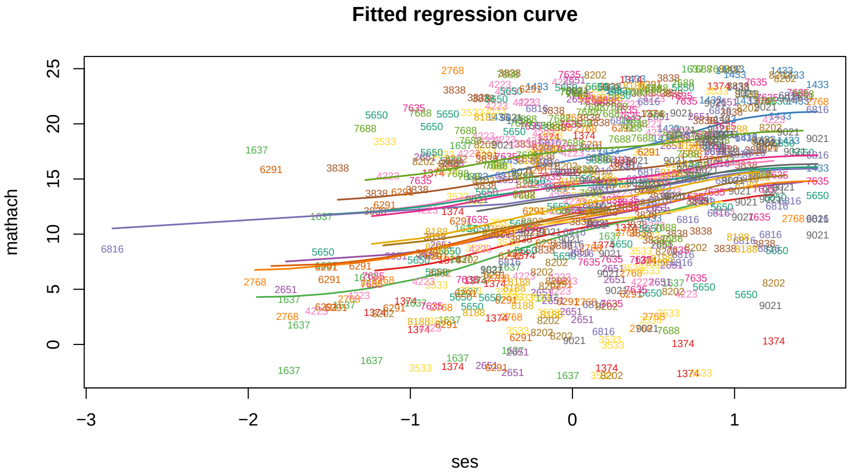
```
plot(
  iprior(mathach ~ ses + schoolid + ses:schoolid, hsbsmall)
)
```



The R/iprior package

```r
plot(
  iprior(mathach ~ . ^ 2, hsbsmall, model = list(kernel = "FBM"))
)
```



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- Compare mean squared errors and log-likelihood values of models.

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##         Canonical      FBM Can. w/ intr FBM w/ intr
## MSE        41.232    40.86       34.809       34.31
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- Other things available:
  - `fitted()` for fitted values.
  - `predict()` for fitted values of a new set of covariates.
  - `resid()` for model residuals.
  - `logLik()` and `deviance()` for model log-likelihood and deviance values respectively.
  - `ipriorOptim()` is a routine which combines EM algorithm and direct optimisation.

The beta I-prior (linear) model

- For "straight line" functions in the Canonical RKHS, its kernel $h_{\boldsymbol{\lambda}} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is defined as

$$h_{\boldsymbol{\lambda}}(\mathbf{x}_i, \mathbf{x}_j) = \sum_{k=1}^{p} \lambda_k x_{ik} x_{jk}$$

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where $\boldsymbol\Lambda = \text{diag}[\lambda_1, \ldots, \lambda_p]$.

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  where $\boldsymbol\Lambda = \text{diag}[\lambda_1, \ldots, \lambda_p]$.
- Putting this into the w I-prior model we have

$$\begin{aligned} \mathbf{y} &= \boldsymbol\alpha + \mathbf{H}_{\boldsymbol\lambda} \mathbf{w} + \boldsymbol\epsilon \\ &= \boldsymbol\alpha + \mathbf{X} \underbrace{\boldsymbol\Lambda \mathbf{X}^\top \mathbf{w}}_{\boldsymbol\beta} + \boldsymbol\epsilon \end{aligned}$$

The beta I-prior (linear) model

- For "straight line" functions in the Canonical RKHS, its kernel $h_{\boldsymbol{\lambda}} : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is defined as

$$\begin{aligned} \mathbf{H}_{\boldsymbol{\lambda}} &= \lambda_1 \mathbf{X}_1 \mathbf{X}_1^\top + \cdots + \lambda_p \mathbf{X}_p \mathbf{X}_p^\top \\ &= \mathbf{X} \boldsymbol{\Lambda} \mathbf{X}^\top, \end{aligned}$$

  where $\boldsymbol{\Lambda} = \operatorname{diag}[\lambda_1, \ldots, \lambda_p]$.
- Putting this into the w I-prior model we have

$$\begin{aligned} \mathbf{y} &= \boldsymbol{\alpha} + \mathbf{H}_{\boldsymbol{\lambda}} \mathbf{w} + \boldsymbol{\epsilon} \\ &= \boldsymbol{\alpha} + \mathbf{X} \underbrace{\boldsymbol{\Lambda} \mathbf{X}^\top \mathbf{w}}_{\boldsymbol{\beta}} + \boldsymbol{\epsilon} \end{aligned}$$

  which implies $\mathrm{E}[\boldsymbol{\beta}] = \mathbf{0}$ and $\mathrm{Var}[\boldsymbol{\beta}] = \psi \boldsymbol{\Lambda} \mathbf{X}^\top \mathbf{X} \boldsymbol{\Lambda}$.

The beta I-prior (linear) model cont.

- The standard multiple regression model with an I-prior on $\boldsymbol{\beta}$

$$
\begin{gathered}
y_i = \alpha + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i \\
\boldsymbol{\beta} \sim \mathrm{N}(\mathbf{0}, \psi \boldsymbol{\Lambda} \mathbf{X}^\top \mathbf{X} \boldsymbol{\Lambda}), \text{ where } \boldsymbol{\Lambda} = \mathrm{diag}[\lambda_1, \ldots, \lambda_p] \\
\epsilon_i \sim \mathrm{N}(0, \psi^{-1}) \\
i = 1, \ldots, n
\end{gathered} \tag{3}
$$

is an equivalent representation of the w I-prior model under the Canonical kernel.

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  is an equivalent representation of the w I-prior model under the Canonical kernel.
- Estimate this model via ML methods as before, or fully Bayes, as we will see soon.

Shrinkage properties of I-priors

- Comparison to ridge regression and Lasso

$$\mathit{Ridge} : \hat{\boldsymbol{\beta}}^R = \arg\min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda \sum_{j=1}^{p} \beta_j^2$$

$$\mathit{Lasso} : \hat{\boldsymbol{\beta}}^L = \arg\min_{\boldsymbol{\beta}} \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + \lambda \sum_{j=1}^{p} |\beta_j|$$

Shrinkage properties of I-priors

- Comparison to ridge regression and Lasso

$$\textit{Ridge} : \beta_1, \dots, \beta_p \sim \mathrm{N}(0, 1/\lambda)$$
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  - After standardising data $\mathbf{X}$, use weakly informative priors

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- I-priors have individual shrinkage coefficients on the $\boldsymbol{\beta}$, and also makes them correlated a priori.

Shrinkage properties of I-priors cont.

Demo

https://haziqjamil.shinyapps.io/iprior/

Full Bayes estimation

- The fully Bayes beta I-prior model is the following hierarchical model

$$
\begin{gathered}
y_i = \alpha + \beta_1 x_{i1} + \cdots + \beta_p x_{ip} + \epsilon_i \\
\epsilon_i \sim \mathrm{N}(0, \psi^{-1}) \\
i = 1, \dots, n \\
\\
\underline{\text{Priors}} \\
\alpha \sim \mathrm{N}(0, a^2) \\
\boldsymbol{\beta} \sim \mathrm{N}(\mathbf{0}, \psi \boldsymbol{\Lambda} \mathbf{X}^\top \mathbf{X} \boldsymbol{\Lambda}), \text{ where } \boldsymbol{\Lambda} = \mathrm{diag}[\lambda_1, \dots, \lambda_p] \\
\psi, \lambda_1^{-2}, \dots, \lambda_p^{-2} \sim \Gamma(c, d)
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\end{gathered}
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- The posterior distribution is

$$
\begin{aligned}
f(\alpha, \boldsymbol{\beta}, \psi, \boldsymbol{\lambda} | \mathbf{y}) &\propto f(\mathbf{y} | \alpha, \boldsymbol{\beta}, \psi, \boldsymbol{\lambda}) f(\alpha, \boldsymbol{\beta}, \psi, \boldsymbol{\lambda}) \\
&\propto f(\mathbf{y} | \alpha, \boldsymbol{\beta}, \psi) f(\alpha) f(\boldsymbol{\beta} | \psi, \boldsymbol{\lambda}) f(\psi) f(\lambda_1) \cdots f(\lambda_p)
\end{aligned}
$$

Estimation using JAGS

- Fit Bayesian models using JAGS (or WinBUGS or OpenBUGS).
- In R, many packages to run JAGS models: `rjags`, `R2Jags`, `runjags`.
- We will use `runjags` as it allows easy parallelisation of chains.
- Simulate a dataset:

```
n <- 100
p <- 2
beta.true <- matrix(c(10, 0), ncol = 1)
X <- matrix(rnorm(n * p, ncol = p)
Y <- X %*% beta.true + rnorm(n, mean = 0, sd = 2)
```

Estimation using JAGS

```
mod <- "
  model {
    for (i in 1:n) {
      Y[i] ~ dnorm(mu[i], psi)
      mu[i] <- alpha + inprod(X[i,1:p], beta[1:p])
    }

    alpha ~ dnorm(0, 0.0001)
    psi ~ dgamma(0.1, 0.0001)
    for (j in 1:p) {
      lambdasq[j] ~ dgamma(0.0001, 0.0001)
      for (k in 1:p) { LambdaInv[j, k] <- equals(j,k) * pow(lambdasq[k], -0.5) }
    }
    BetaPrec <- LambdaInv[1:p, 1:p] %*% XTX.inv %*% LambdaInv[1:p, 1:p] / psi
    beta[1:p] ~ dmnorm(rep(0, p), BetaPrec)

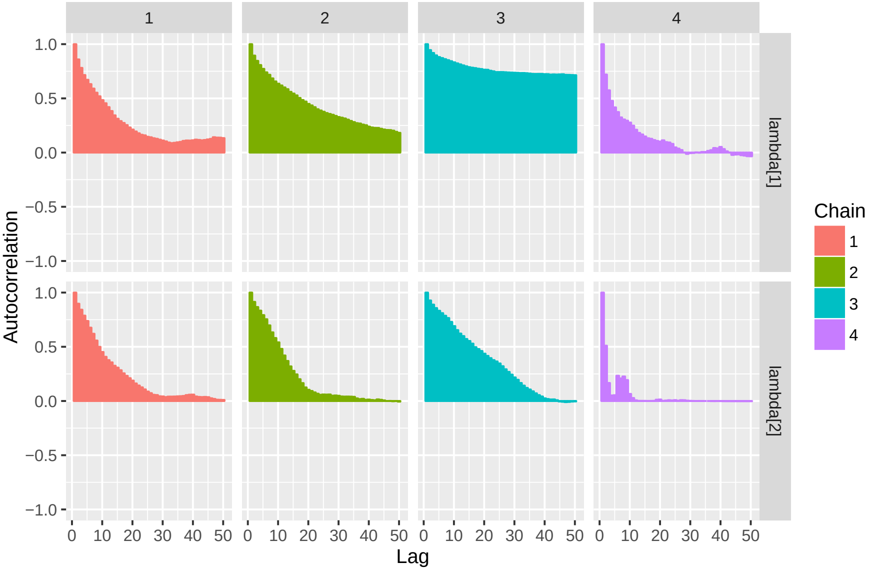
    sigma <- pow(psi, -0.5)
    lambda[1:p] <- pow(lambdasq[1:p], 0.5)
  }
  #data# Y, X, XTX.inv, n, p
  #inits# alpha, beta, psi, lambdasq
  #monitor# alpha, beta, sigma, lambda
"
```

Estimation using JAGS

```
(mod.fit <- run.jags(mod, n.chains = 4, sample = 2500, thin = 10,
                     method = "parallel", n.sims = 4))


##
## JAGS model summary statistics from 10000 samples (thin = 10; chains = 4; adapt+b
##
##                Lower95      Median    Upper95       Mean        SD         Mode
## alpha         -0.39905   -0.053978    0.36319  -0.052545   0.19233    -0.039251
## beta[1]         9.3746      9.7564     10.134     9.7574   0.19342       9.7704
## beta[2]      -0.010512  2.8816e-30   0.020854  0.0033068  0.030077   5.9629e-23
## sigma           1.6469      1.8978     2.1805     1.9044   0.13755       1.8887
## lambda[1]      0.55642      2.7259     16.499     4.6509    5.0124       1.7294
## lambda[2]   1.0291e-77  1.4207e-21  0.0052381  0.0018802  0.012068   3.0584e-23
##
##                  MCerr MC%ofSD SSeff     AC.100   psrf
## alpha        0.0019229       1 10003   0.014252 1.0008
## beta[1]      0.0019342       1 10000   0.020871 0.9999
## beta[2]      0.0008697     2.9  1196    0.10176 1.0591
## sigma        0.0013755       1 10000 -0.0037105 1.0004
## lambda[1]      0.26974     5.4   345    0.53237 1.0284
## lambda[2]   0.00067477     5.6   320    0.39277 1.2695
##
## Total time taken: 10.2 seconds
```

Estimation using JAGS



Estimation using JAGS

Problems

- Trace plot of λ_k can be very erratic, and samples found to be severely autocorrelated.
- Since the scale parameters are very important for Bayesian Variable Selection, it is imperative that these are estimated correctly.
- Suggestions:
  - Improve samples - Hamiltonian Monte Carlo?
  - Treat $\boldsymbol{\lambda}$ as fixed, replacing them with estimates obtained using ML methods.

Introduction

- Introduced as Hybrid Monte Carlo [Duane et al., 1987] for use in lattice models of quantum theory. Statistical applications started appearing sparsely in the 1990s.
- Development of HMC software (Stan) began in 2011, motivated by the difficulties faced when doing full Bayesian inference on multilevel generalised linear models.
- The basic idea behind HMC is to use Hamiltonian dynamics to propose new states, instead of "random walks".

$$\mathbf{x} \xrightarrow[\text{Markov Transition}]{} \mathbf{x}^*$$

- High probability of acceptance
- Distant move

Hamiltonian dynamics

- A reformulation of classical mechanics which describes motion through Hamilton's equations:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \frac{\partial H}{\partial \mathbf{p}} \quad \text{and} \quad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial H}{\partial \mathbf{x}},$$

where $H = H(\mathbf{x}, \mathbf{p})$ is the Hamiltonian of the system (total energy), and $(\mathbf{x}, \mathbf{p})$ are the position and momentum coordinates of the body in motion.

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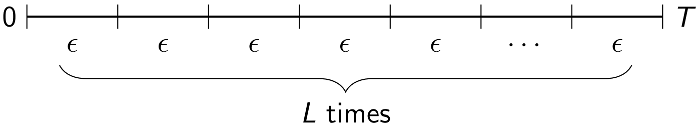
Hamiltonian dynamics cont.

- To describe the evolution of $\big(\mathbf{x}(t), \mathbf{p}(t)\big)$ from time t to $t+T$, it is necessary to discretise time and split $T = L \cdot \epsilon$.



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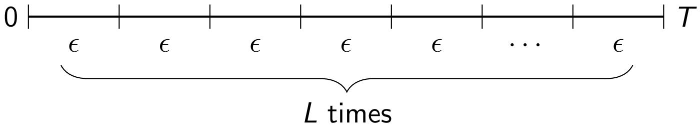

- Solve the system of differential equations using Euler's method, or the more commonly used leapfrog integration:

$$\text{Step 1: } \mathbf{p}(t + \epsilon/2) = \mathbf{p}(t) - \frac{\epsilon}{2} \cdot \frac{\partial}{\partial \mathbf{x}} U\big(\mathbf{x}(t)\big)$$

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\text{Step 3:} \quad \mathbf{p}(t+\epsilon) &= \mathbf{p}(t+\epsilon/2) - \frac{\epsilon}{2} \cdot \frac{\partial}{\partial \mathbf{x}} U\big(\mathbf{x}(t+\epsilon)\big)
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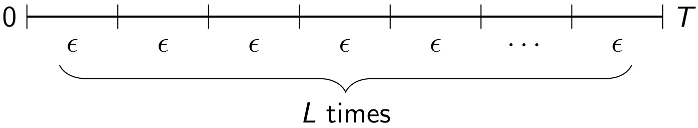

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Steps 1-3 are repeated L times.

Hamiltonian dynamics cont.

Demo

`https://haziqjamil.shinyapps.io/hmc1/`

Probability and the Hamiltonian

- Given some energy function $E(\boldsymbol{\theta})$ over states $\boldsymbol{\theta}$, the *canonical distribution* of the states $\boldsymbol{\theta}$ is given by the pdf

$$f(\boldsymbol{\theta}) = \frac{1}{Z} \exp\left[-\frac{E(\boldsymbol{\theta})}{kT}\right].$$

where k is Boltzmann's constant, T is the absolute temperature of the system, and Z is a normalising constant.

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- Typically, choose T such that $kT = 1$.

Choosing the energy functions

- Using a *quadratic kinetic energy function* $K(\mathbf{p}) = \mathbf{p}^\top \mathbf{M}^{-1}\mathbf{p}/2$ yields the probability density function

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$$U(\mathbf{x}) = -\log f(\mathbf{x}),$$

  since $f(\mathbf{x}) \propto \exp[-U(\mathbf{x})]$, where $f(\mathbf{x})$ is the target density from which we wish to sample.

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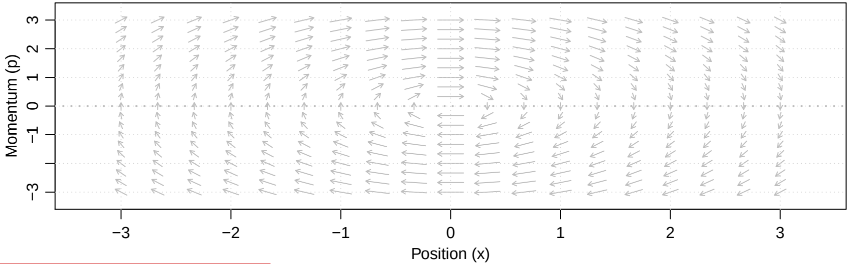

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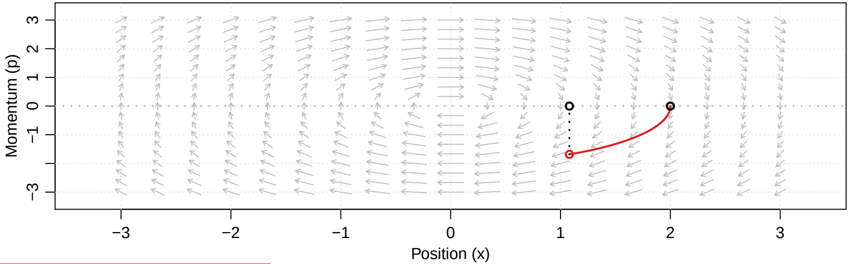
  Step 2 *Metropolis update*. Simulate Hamiltonian dynamics using L leapfrogs of step-size ϵ and obtain a new state $(\mathbf{x}^*, \mathbf{p}^*)$. Accept the proposal state with probability $\min(1, A)$, where

$$A = \frac{f(\mathbf{x}^*, \mathbf{p}^*)}{f(\mathbf{x}, \mathbf{p})} = \exp\left[H(\mathbf{x}, \mathbf{p}) - H(\mathbf{x}^*, \mathbf{p}^*)\right].$$



Hamiltonian Monte Carlo

- To sample variables $\mathbf{x}$, introduce momentum variables $\mathbf{p}$ and sample jointly from $f(\mathbf{x}, \mathbf{p}) = f(\mathbf{x})f(\mathbf{p})$.
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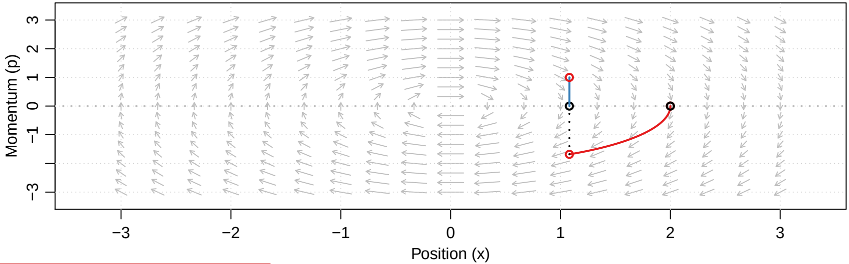

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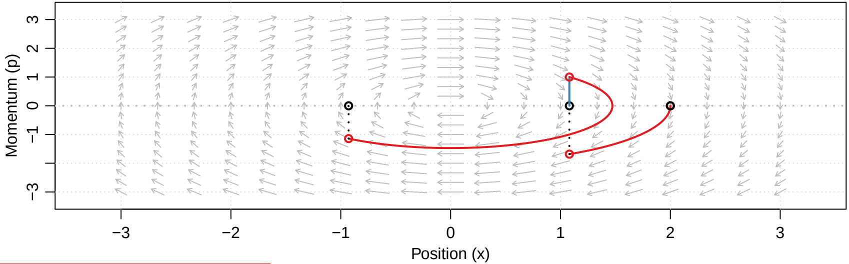

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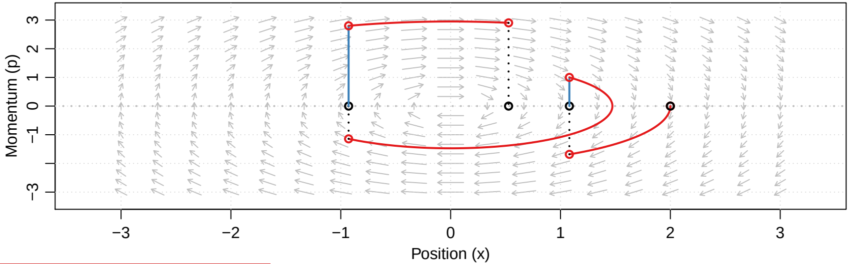

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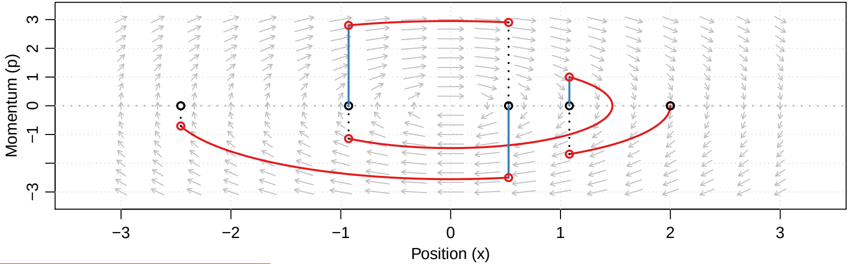

Hamiltonian Monte Carlo cont.

Demo

https://haziqjamil.shinyapps.io/hmc2/

Stan

`http://mc-stan.org`

- Stan interfaces: R, Python, shell, MATLAB, Julia, Stata, and Mathematica. Runs on Linux, Mac and Windows.
- R package `rstan` uses Stan modelling language. For expression-based Bayesian regression modelling, package `rstanarm` is available.
- Nice things about Stan
  - Tuning is done automatically.
  - Vast library of differentiable probability functions, or code your own.
  - Conjugacy has no computational advantage.
  - Optimising for efficiency possible, e.g. vectorisation.

Stan example

```
stan.iprior.mod <- "
  function {
    ...
  }
  data {
    int n; // number of data
    int p; // number of parameters
    vector[n] Y; // responses
    matrix[n, p] X; // (centred) data
  }
  transformed data {
    matrix[p, p] XTX;
    XTX = X' * X;
  }
  parameters {
    real alpha;  // intercept
    real<lower=0> sigma;  // s.d. of errors
    vector[p] beta;  // regression coefficients
    vector<lower=0>[p] lambda;  // I-prior scale parameters
  }
```

Stan example

```
transformed parameters {
  vector[p] lambdasq;
  cov_matrix[p] Sigma;
  vector[n] mu;
  lambdasq = lambda .* lambda;
  Sigma = diag_matrix(lambda) * XTX * diag_matrix(lambda) ./ (sigma ^ 2);
  mu = alpha + X * beta;
}
model {
  target += inv_gamma_lpdf(lambdasq | 0.0001, 0.0001);
  target += multi_normal_lpdf(beta | rep_vector(0, p), Sigma);
  target += normal_lpdf(Y | mu, sigma);
}
generated quantities {
  ...
}
"
```

Stan example

- Compile the Stan model.

```
m <- stan_model(model_code = stan.mod)
m@model_name <- "iprior"
```

Stan example

- Compile the Stan model.

```
m <- stan_model(model_code = stan.mod)
m@model_name <- "iprior"
```

- Set the data for Stan to use.

```
stan.dat <- list(Y = as.vector(Y), X = Xs, n = n, p = p)
```

Stan example

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m@model_name <- "iprior"
```

- Set the data for Stan to use.

```
stan.dat <- list(Y = as.vector(Y), X = Xs, n = n, p = p)
```

- Begin sampling

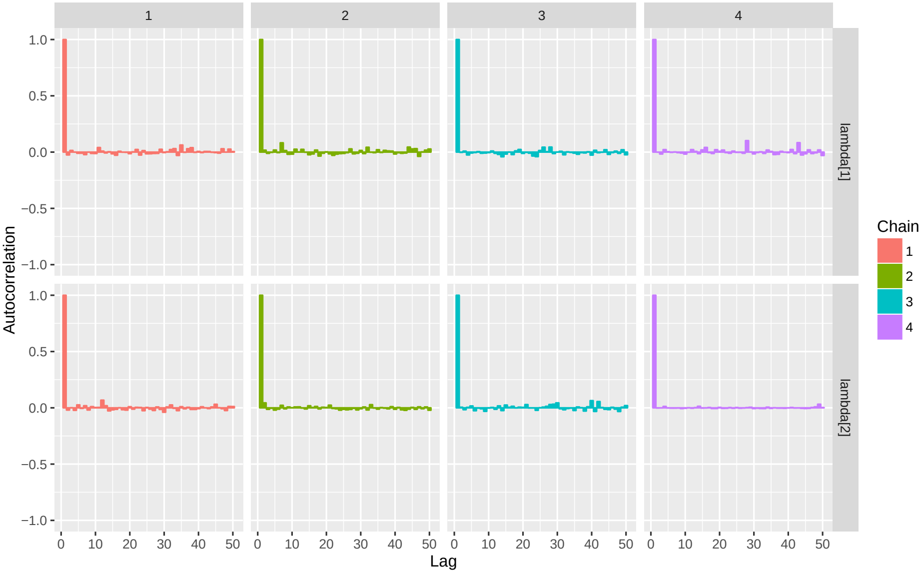
```
fit.stan <- stan(model_code = stan.mod, data = stan.dat,
                 pars = c("alpha", "beta", "lambda", "sigma"),
                 iter = 50000, chains = 4, thin = 10)
```

Stan example

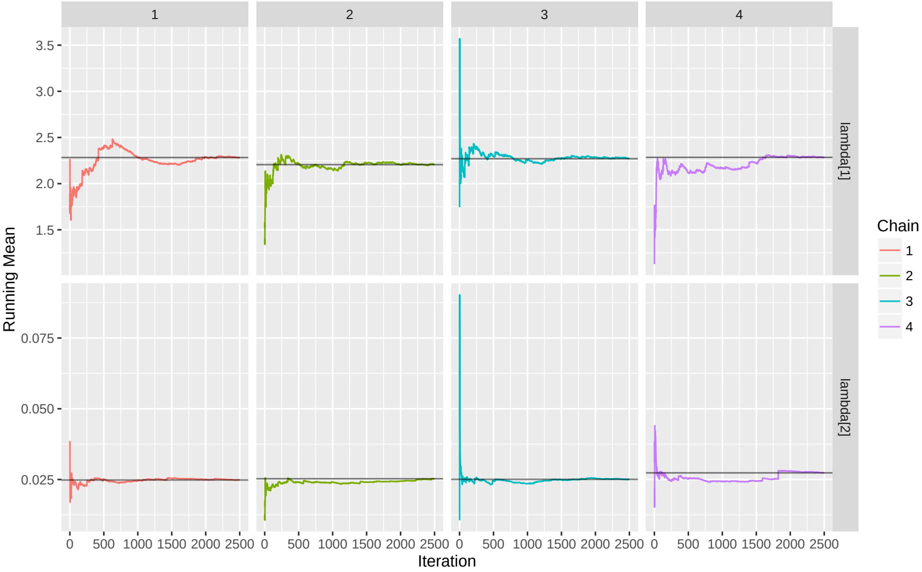
```
print(fit.stan)

## Inference for Stan model: iprior.
## 4 chains, each with iter=50000; warmup=25000; thin=10;
## post-warmup draws per chain=2500, total post-warmup draws=10000.
##
##                mean se_mean   sd    2.5%     25%     50%     75%   97.5%
## alpha         -1.04    0.00 0.19   -1.40   -1.16   -1.04   -0.92   -0.68
## beta[1]        9.71    0.00 0.20    9.32    9.58    9.71    9.84   10.10
## beta[2]        0.07    0.00 0.10   -0.10    0.01    0.06    0.12    0.31
## lambda[1]      2.26    0.03 2.55    0.70    1.14    1.61    2.47    7.78
## lambda[2]      0.03    0.00 0.06    0.01    0.01    0.02    0.03    0.09
## sigma          1.91    0.00 0.13    1.68    1.82    1.91    2.00    2.20
## lp__        -224.20    0.02 1.85 -228.60 -225.24 -223.88 -222.82 -221.62
##             n_eff Rhat
## alpha       10000    1
## beta[1]     10000    1
## beta[2]      9410    1
## lambda[1]   10000    1
## lambda[2]    9972    1
```

Stan example



Stan example



HMC unable to sample from discrete distributions

- HMC requires that the domain of $f(\mathbf{x})$ is continuous and $\partial \log f(\mathbf{x}) / \partial \mathbf{x}$ is inexpensive to compute.
- This is a problem for our Bayesian Variable Selection model because we need posterior samples of $\gamma \in \{0, 1\}^p$.
- Three ideas:
  - Marginalise the discrete variables.
  - Use an underlying latent continuous variable.
  - Augment with Gibbs sampling.

Approach 1: Marginalise

- Let $\boldsymbol{\theta}$ be some continuous parameters and γ be some discrete parameters in the model with data $\mathbf{y}$.
- Since unable to sample from $f(\gamma|\mathbf{y})$, integrate out γ from the model, and just sample from the posterior of $\boldsymbol{\theta}$

$$f(\boldsymbol{\theta}|\mathbf{y}) = \sum_{\gamma} f(\boldsymbol{\theta}, \gamma|\mathbf{y}) = f(\boldsymbol{\theta}) \sum_{\gamma} f(\mathbf{y}|\boldsymbol{\theta}, \gamma) f(\gamma)$$

- The unnormalised posterior probability mass function for γ is

$$q(\gamma) = \frac{1}{M} \sum_{m=1}^{M} f(\boldsymbol{\theta}^{(m)}, \gamma|\mathbf{y})$$

  where $m = 1, \ldots, M$ is the index for the posterior draws.
- *Problem: For Bayesian Variable Selection models, this is intractable because need to sum over all 2^p models.*

Approach 2: Latent continuous variables

- For the Bayesian Variable Selection model, assume there is underlying standard normal random variable Z_j for each $j = 1, \dots, p$ such that

$$\gamma_j = \begin{cases} 1 & Z_j \geq 0 \\ 0 & Z_j < 0 \end{cases}$$

- Probabilities are preserved: $\text{P}[\gamma_j = 1] = \text{P}[Z_j \geq 0] = 0.5$.
- *Problems:*
  - *Does this make sense?*
  - *The discrete variables still "exist", so possibly derivatives will break.*

Approach 3: Use Gibbs sampler

- Sample the continuous parameters $\boldsymbol{\theta}$ using HMC.
- At each iteration m, use $\boldsymbol{\theta}^{(m)}$ in the Gibbs conditional densities to sample γ.
- *Problem: Have to write code for the HMC sampler, which won't include all the automatic tuning that Stan has.*

Summary

- For our I-prior Bayesian Variable Selection model
  - Promising results in both simulated and real-world data.
  - The individual scale parameters $\lambda_1, \ldots, \lambda_p$ are important.
  - We have used ML estimate for $\boldsymbol{\lambda}$ in our Bayesian model.

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  - Promising results in both simulated and real-world data.
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- To-do list:
  - Any model consistency results for Bayesian variable selection models?
  - Any mathematical justification as to why we should use individual scale parameters?
  - Does the off-diagonal elements in the I-prior covariance matrix affect variable selection results in multicollinearity situations?

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  - Does the off-diagonal elements in the I-prior covariance matrix affect variable selection results in multicollinearity situations?
- Wishlist: Make HMC work for Bayesian variable selection models.

What we've seen today

1. I-prior models estimated using ML methods (EM algorithm) and use of the `iprior` package in R.
2. Shrinkage properties of I-priors for use in Bayesian variable selection.
3. Bayesian estimation in JAGS.
4. Shiny apps for reactive programming.
5. Hamiltonian dynamics and Hamiltonian Monte Carlo.
6. Bayesian inference using HMC via Stan.
7. `knitr` for combining (evaluated) R code and plots into documents.
8. Git and GitHub for version control.

knitr example

- You type:

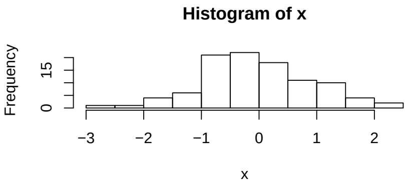
```
<<chunk.name, echo = TRUE>>=
x <- rnorm(100)
max(x)
hist(x)
@
```

- The output:

```r
x <- rnorm(100)
max(x)

## [1] 2.375356
```

```r
hist(x)
```



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End

Thank you!

7 Additional material

`lme4` methods

MLE vs Bayes for scale parameters

Minimising profiled deviance (à la `lme4`)

- Very fast algorithm to obtain MLEs of mixed-effects models by using sparse Cholesky decomposition.
- Consider the mixed-effects model

$$
\begin{gathered}
\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\mathbf{b} + \boldsymbol{\epsilon} \\
\boldsymbol{\epsilon} \sim \mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I}_n) \\
\mathbf{b} \sim \mathrm{N}(\mathbf{0}, \boldsymbol{\Sigma})
\end{gathered}
$$

- Suppose that $\boldsymbol{\Sigma} = \sigma^2 \boldsymbol{\Lambda}_{\boldsymbol{\theta}} \boldsymbol{\Lambda}_{\boldsymbol{\theta}}^\top$. Then the following model is equivalent, where we have used the subsitution $\mathbf{b} = \boldsymbol{\Lambda}_{\boldsymbol{\theta}} \mathbf{u}$:

$$
\begin{gathered}
\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{Z}\boldsymbol{\Lambda}_{\boldsymbol{\theta}}\mathbf{u} + \boldsymbol{\epsilon} \\
\boldsymbol{\epsilon} \sim \mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I}_n) \\
\mathbf{u} \sim \mathrm{N}(\mathbf{0}, \sigma^2 \mathbf{I}_n)
\end{gathered}
$$

Minimising profiled deviance (à la `lme4`) cont.

- The density of interest is $f(\mathbf{y}) = \int h(\mathbf{u})\, \mathrm{d}\mathbf{u}$, where

$$
\begin{aligned}
h(\mathbf{u}) &= f(\mathbf{y}|\mathbf{u}) f(\mathbf{u}) \\
&= (2\pi\sigma^2)^{-(n+q)/2} \exp\left[- \frac{\|\mathbf{y} - \mathbf{X}\beta - \mathbf{Z}\boldsymbol{\Lambda}_\theta \mathbf{u}\|^2 + \|\mathbf{u}\|^2}{2\sigma^2} \right]
\end{aligned}
$$

Minimising profiled deviance (à la `lme4`) cont.

- The density of interest is $f(\mathbf{y}) = \int h(\mathbf{u})\,\mathrm{d}\mathbf{u}$, where

$$h(\mathbf{u}) = f(\mathbf{y}|\mathbf{u})f(\mathbf{u})$$
$$= (2\pi\sigma^2)^{-(n+q)/2} \exp\left[-\frac{\|\mathbf{y} - \mathbf{X}\beta - \mathbf{Z}\boldsymbol{\Lambda}_{\boldsymbol{\theta}}\mathbf{u}\|^2 + \|\mathbf{u}\|^2}{2\sigma^2}\right]$$

- Each calculation of $f(\mathbf{y})$ involves obtaining the conditional modes

$$\tilde{\mathbf{u}}(\boldsymbol{\theta}, \boldsymbol{\beta}) = \arg\min_{\mathbf{u}} d(\mathbf{u}, \boldsymbol{\theta}, \boldsymbol{\beta})$$

by computing the sparse Cholesky factorisation

$$\mathbf{L}_{\boldsymbol{\theta}}\mathbf{L}_{\boldsymbol{\theta}}^\top = \boldsymbol{\Lambda}_{\boldsymbol{\theta}}^\top \mathbf{Z}^\top \mathbf{Z}\boldsymbol{\Lambda}_{\boldsymbol{\theta}} + \mathbf{I}_q,$$

and solving $\mathbf{L}_{\boldsymbol{\theta}}^\top \tilde{\mathbf{u}} = c(\boldsymbol{\theta}, \boldsymbol{\beta})$ by back substitution.

Minimising profiled deviance (à la `lme4`) cont.

- For linear mixed models, $f(\mathbf{y}) = \int h(\mathbf{u})\,\mathrm{d}\mathbf{u}$ has a closed-form expression in terms of $\mathbf{L}_{\boldsymbol\theta}$ and $\tilde{\mathbf{u}}(\boldsymbol\theta, \boldsymbol\beta)$:

$$f(\mathbf{y}) = (2\pi\sigma^2)^{-n/2}|\mathbf{L}_{\boldsymbol\theta}|^{-1} \exp\left[-\frac{d(\tilde{\mathbf{u}}, \boldsymbol\theta, \boldsymbol\beta)}{2\sigma^2}\right]. \tag{5}$$

- On the deviance scale, we have $D(\boldsymbol\theta, \boldsymbol\beta, \sigma) = -2\log f(\mathbf{y})$. The value of σ which minimises the deviance is

$$\sigma^2(\boldsymbol\theta, \boldsymbol\beta) = \frac{d(\tilde{\mathbf{u}}, \boldsymbol\theta, \boldsymbol\beta)}{n}.$$

- Plugging this back into (5), we obtain the profiled deviance

$$D(\boldsymbol\theta, \boldsymbol\beta) = 2\log|\mathbf{L}_{\boldsymbol\theta}| + n\left(1 + \log\left(2\pi\frac{d(\tilde{\mathbf{u}}, \boldsymbol\theta, \boldsymbol\beta)}{n}\right)\right)$$

which is then minimised to obtain MLEs $\hat{\boldsymbol\theta}$, $\hat{\boldsymbol\beta}$ and $\sigma^2(\hat{\boldsymbol\theta}, \hat{\boldsymbol\beta})$.

Minimising profiled deviance (à la `lme4`) cont.

- "Eliminate" fixed effects $\boldsymbol{\beta}$.
  - Find conditional modes $\tilde{\boldsymbol{\beta}}(\boldsymbol{\theta})$

$$\begin{pmatrix} \tilde{\mathbf{u}}(\boldsymbol{\theta}) \\ \tilde{\boldsymbol{\beta}}(\boldsymbol{\theta}) \end{pmatrix} = \operatorname*{arg\,min}_{(\mathbf{u},\boldsymbol{\beta})} d(\mathbf{u}, \boldsymbol{\beta}, \boldsymbol{\theta})$$

via a sparse Cholesky decomposition. Following a similar method as before, obtain a profiled deviance which depends only on $\boldsymbol{\theta}$

$$D(\boldsymbol{\theta}) = 2 \log |\mathbf{L}_{\boldsymbol{\theta}}| + n \left(1 + \log \left(2\pi \frac{d(\tilde{\mathbf{u}}, \boldsymbol{\theta}, \tilde{\boldsymbol{\beta}})}{n} \right) \right).$$

Minimising profiled deviance (à la `lme4`) cont.

- "Eliminate" fixed effects $\boldsymbol\beta$.
  - Find conditional modes $\tilde{\boldsymbol\beta}(\boldsymbol\theta)$

$$\begin{pmatrix} \tilde{\mathbf{u}}(\boldsymbol\theta) \\ \tilde{\boldsymbol\beta}(\boldsymbol\theta) \end{pmatrix} = \underset{(\mathbf{u},\boldsymbol\beta)}{\arg\min}\, d(\mathbf{u},\boldsymbol\beta,\boldsymbol\theta)$$

    via a sparse Cholesky decomposition. Following a similar method as before, obtain a profiled deviance which depends only on $\boldsymbol\theta$

$$D(\boldsymbol\theta) = 2\log|\mathbf{L}_{\boldsymbol\theta}| + n\left(1 + \log\left(2\pi\frac{d(\tilde{\mathbf{u}},\boldsymbol\theta,\tilde{\boldsymbol\beta})}{n}\right)\right).$$

  - In addition, use the restricted maximum likelihood (REML) criterion

$$D_R(\boldsymbol\theta,\sigma) = -2\log\int f(\mathbf{y})\,\mathrm{d}\boldsymbol\beta.$$

    Again, follow similar steps to obtain the profiled REML criterion

$$D_R(\boldsymbol\theta) = 2\log(|\mathbf{L}_{\boldsymbol\theta}|\mathbf{L}_{\mathbf{X}}|) + (n-p)\left(1 + \log\left(2\pi\frac{d(\tilde{\mathbf{u}},\boldsymbol\theta,\tilde{\boldsymbol\beta})}{n-p}\right)\right).$$

Coerce the w I-prior model into a mixed-model

$$
\begin{aligned}
\mathbf{y} &= \boldsymbol{\alpha} + (\lambda_1 \mathbf{H}_1 + \cdots + \lambda_p \mathbf{H}_p)\mathbf{w} + \boldsymbol{\epsilon} \\
&= \underbrace{\begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}}_{\mathbf{X}} \underbrace{\begin{bmatrix} \alpha \end{bmatrix}}_{\beta} + \underbrace{\begin{bmatrix} \mathbf{H}_1 & \cdots & \mathbf{H}_p \end{bmatrix}}_{\mathbf{Z}} \underbrace{\begin{bmatrix} \lambda_1 \mathbf{I}_n \\ \vdots \\ \lambda_p \mathbf{I}_n \end{bmatrix}}_{\mathbf{\Lambda}_\lambda} \mathbf{w} + \boldsymbol{\epsilon} \\
&= \mathbf{X}\beta + \mathbf{Z}\mathbf{\Lambda}_\lambda \mathbf{w} + \boldsymbol{\epsilon} \\
&= \mathbf{X}\beta + \mathbf{Z} \underbrace{\left(\frac{1}{\sigma^2} \mathbf{\Lambda}_\lambda \right)}_{\mathbf{\Lambda}_\theta} \underbrace{(\sigma^2 \mathbf{w})}_{\mathbf{u}} + \boldsymbol{\epsilon} \\
&= \mathbf{X}\beta + \mathbf{Z}\mathbf{\Lambda}_\theta \mathbf{u} + \boldsymbol{\epsilon}
\end{aligned}
$$

- Our scale parameters are contained in $\boldsymbol{\theta} = (\lambda_1/\sigma^2, \dots, \lambda_p/\sigma^2)$.
- *Problem: Our* **Z** *matrix is dense, so not able to use sparse Cholesky methods.*

MLE vs Bayes for scale parameters

- For each $k = 1, \dots, p$, the maximum a posteriori (MAP) estimate is

$$\begin{aligned}\hat\lambda_k^{MAP} &= \arg\max_{\lambda_k} f(\alpha, \boldsymbol\beta, \psi, \boldsymbol\lambda | \mathbf{y}) \\ &= \arg\max_{\lambda_k} f(\mathbf{y}, \boldsymbol\beta | \alpha, \psi, \boldsymbol\lambda) f(\psi) f(\lambda_1) \cdots f(\lambda_p) \\ &= \arg\max_{\lambda_k} f(\mathbf{y}, \boldsymbol\beta | \alpha, \psi, \boldsymbol\lambda) f(\lambda_k)\end{aligned}$$

  whereas the ML estimate is

$$\begin{aligned}\hat\lambda_k^{ML} &= \arg\max_{\lambda_k} f(\mathbf{y}; \boldsymbol\lambda, \psi) \\ &= \arg\max_{\lambda_k} \int f(\mathbf{y}, \boldsymbol\beta; \boldsymbol\lambda, \psi) \, \mathrm{d}\boldsymbol\beta\end{aligned}$$

- $\hat\lambda_k^{MAP} = \hat\lambda_k^{ML}$ if the beta I-prior model is marginalised over $\boldsymbol\beta$, and a uniform prior is used for each λ_k.

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