Bayesian Regression Trees STAT8810, Fall 2017

M.T. Pratola

October 17, 2017

Today



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 - Local models depend on subset of the data, increasing computational scalability compared to GP regression.
- Tradeoff is model no longer interpolates observations.
 - Fine for data which is observed with obserational error.
 - Not ideal for deterministic simulator outputs, but we already know approximations of various sorts are needed for this problem.

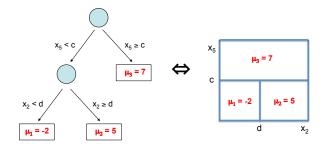


Figure 1: A Single Tree with Scalar Terminal Nodes

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- To take a Bayesian approach, we need to define a stochastic representation of this model.
- Let us call $z(\mathbf{x}) : \mathbb{R}^d \to \mathbb{R}$ for $\mathbf{x} \in \mathbb{R}^d$ to be a mapping from the inputs to the (unobserved) response function.
- And let us assume that the observed data, y(x_i), i = 1,..., n is observed with i.i.d. Normally distributed error,

$$y(\mathbf{x}_i) = z(\mathbf{x}_i) + \epsilon_i, \ \ \epsilon_i \sim N(0, \sigma^2).$$

- Previously, in the GP approach, we would place a GP prior on the $z(\mathbf{x})$ process and write the posterior of the parameters, ρ , as

$$\pi(oldsymbol{
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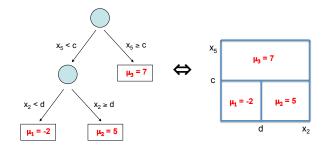
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 - Model complexity?

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- A realization of $Z(\mathbf{x}|\mathcal{T}, \mathcal{M})$ is this:



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- Our task then is to specify priors on \mathcal{T}, \mathcal{M} and derive an algorithm for sampling the posterior distribution of these parameters given data.
 - Presumably, if our model definition is useful, we will be able to predict our observations fairly well.

• What parameters are associated with the abstract representation \mathcal{T} ?

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 - For each terminal node η_j , there is an associated scalar parameter μ_j .
- There are many ways one might specify a stochastic tree model using these variables. We follow the generative process described in a series of papers by Chipman, George and McCulloch (CGM)[†].

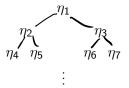
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- Another way of saying this is that tree models are not arbitrary graphical models where one might learn both the η_i 's and the e_{ij} 's.
- For simplicity, a unique numbering system for nodes is employed. η₁ is the root node, and the expansion looks like:



Priors

 Let *I* represent the collection of indices of internal nodes η_i, and *B* represent the collection of indices of terminal nodes η_i.

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M.T. Pratola: Efficient Metropolis-Hastings Proposal Mechanisms for Bayesian

- Let *I* represent the collection of indices of internal nodes η_i, and *B* represent the collection of indices of terminal nodes η_i.
- The CGM prior† is as follows:

$$\pi(\sigma^{2}, \mathcal{T}, \mathcal{M}) = \pi(\sigma^{2})\pi(\mathcal{M}|\mathcal{T})\pi(\mathcal{T})$$

$$= \pi(\sigma^{2})\prod_{j\in\mathcal{B}}\pi(\mu_{j}|\eta_{j})\pi(\eta_{j} \text{ is terminal})$$

$$\times \prod_{k\in\mathcal{I}}\pi(v_{k}, c_{k}|\mathcal{T}\setminus\eta_{k})\pi(\eta_{k} \text{ is internal})$$

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• The prior on a node being internal/terminal is given by the so-called depth penalizing prior,

$$\pi(\eta_j \text{ is internal}) = lpha (1 + d(\eta_j, \eta_1))^{-eta}$$

where $d(\eta_j, \eta_1)$ is the depth of node $\eta_j, \alpha \in (0, 1)$ and $\beta \in [0, \infty)$, and correspondingly,

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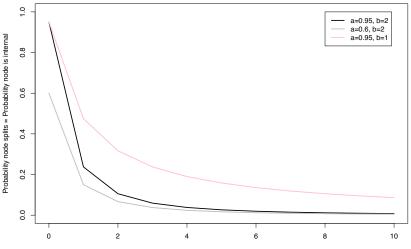
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$$\pi(\eta_j \text{ is terminal}) = 1 - \pi(\eta_j \text{ is internal}).$$

 Interpretation is probability a node splits (and is hence internal) decreases the deeper that node is in the tree. In other words, this prior favors shallower, sparser trees.





Depth of node

• The prior on cutpoints *c_i* is typically a discrete uniform distribution over the cutpoints

$$\left\{0,\frac{1}{n_v-1},\ldots,\frac{n_v-2}{n_v-1},1\right\}$$

where n_v is a fixed, user-specified discretization resolution for variable v.

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• The prior on variables *v_i* is typically a discrete uniform distribution over the variable indices

$$\{1,2,\ldots,d\}.$$

• The prior on the terminal node scalar parameters are i.i.d. conjugate normal,

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 this is a different, but still conjugate, prior than what we had used in our GP model (where we used precision λ ~ Gamma).

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 - If node 2 is internal, draw v_2 and c_2 from Uniform priors[†].
- 3. etc.

```
set.seed(88)
cuts=seq(0.1,0.9,length=9)
nonterms=c()
terms=c()
stop=FALSE
alpha=0.95
beta=2
# Node 1
d=0
psplit=alpha*(1+d)^(-beta)
runif(1)<psplit</pre>
```

[1] TRUE

nonterms=c(1)

```
# Nodes 2,3
d=1
# Node 2
psplit=alpha*(1+d)^(-beta)
runif(1)<psplit</pre>
```

[1] TRUE

```
nonterms=c(nonterms,2)
# Node 3
psplit=alpha*(1+d)^(-beta)
runif(1)<psplit</pre>
```

[1] FALSE

terms=c(3)

Nodes 4,5
d=2
Node 4
psplit=alpha*(1+d)^(-beta)
runif(1)<psplit</pre>

[1] FALSE

```
terms=c(terms,4)
# Node 5
psplit=alpha*(1+d)^(-beta)
runif(1)<psplit</pre>
```

[1] FALSE

```
terms=c(terms,5)
# Nowhere left to grow
```

Now select variable, cutpoints for internal nodes
Since we have only 1 variable, its always used in splits
variables=rep(0,length(nonterms))

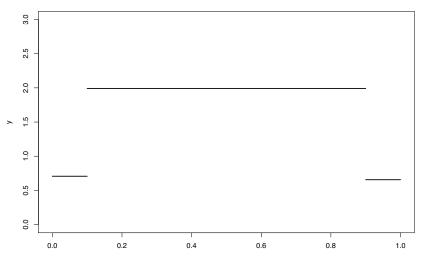
Now get cuts
cutpoints=rep(0,length(nonterms))
cutpoints[1]=sample(cuts,1)
cutpoints[1]

[1] 0.9

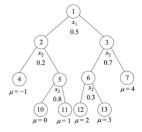
Now get cut for node 2
cuts=cuts[cuts<cutpoints[1]]
cutpoints[2]=sample(cuts,1)
cutpoints[2]</pre>

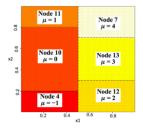
[1] 0.1

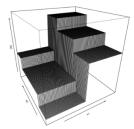
Now draw terminal node parameters from N(0,tau²)
tau2=1
mu=rep(0,length(terms))
for(i in 1:length(terms))
 mu[i]=rnorm(1,mean=0,sd=sqrt(tau2))



Example Realization with 2 predictors[†]

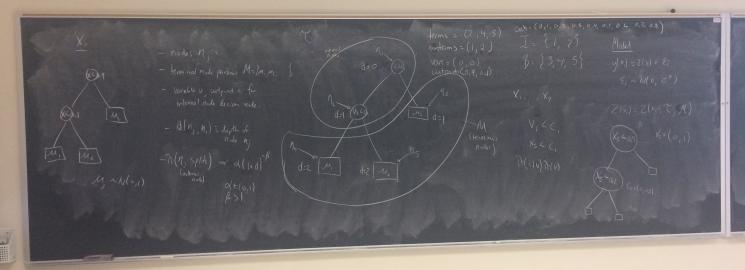






Three different views of a bivariate single tree.

† Source: E.I. George, BNPSKi (2014).



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• Given observations $\mathbf{y} = (y_1, \dots, y_n)$, we are interested in sampling the posterior distribution

$$\pi(\sigma^2, \mathcal{T}, \mathcal{M} | \mathbf{y}) \propto L(\sigma^2, \mathcal{T}, \mathcal{M} | \mathbf{y}) \pi(\sigma^2) \pi(\mathcal{M} | \mathcal{T}) \pi(\mathcal{T})$$

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 Conditional on a realization of our stochastic tree process, our likelihood function is

$$L(\sigma^{2}, \mathcal{T}, \mathcal{M} | \mathbf{y}) = \frac{1}{\sqrt{2\pi}\sigma^{n}} exp\left(-\frac{1}{2\sigma^{2}} \sum_{i=1}^{n} (y_{i} - z(\mathbf{x}_{i}))^{2}\right)$$

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- We'll go in reverse order...

Draw $\sigma^2 | \mathcal{T}, \mathcal{M}, \mathbf{y}$

• We have

$$\pi(\sigma^{2}|\nu,\tau^{2}) = \frac{\left(\frac{\nu\tau^{2}}{2}\right)^{\nu/2}}{\Gamma\left(\frac{\nu}{2}\right)\sigma^{\nu+2}} \exp\left(-\frac{\nu\tau^{2}}{2\sigma^{2}}\right) \propto \frac{1}{\sigma^{\nu+2}} \exp\left(-\frac{\nu\tau^{2}}{2\sigma^{2}}\right)$$

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So,

$$\pi(\sigma^{2}|\mathcal{T}, \mathcal{M}, \mathbf{y}) \propto \frac{1}{\sigma^{n}} exp\left(-\frac{1}{2\sigma^{2}} \sum_{i=1}^{n} (y_{i} - z(\mathbf{x}_{i}))^{2}\right)$$
$$\times \frac{1}{\sigma^{\nu+2}} exp\left(-\frac{\nu\tau^{2}}{2\sigma^{2}}\right)$$
$$= \frac{1}{\sigma^{(\nu+n)+2}} exp\left(-\frac{(\nu+n)}{2\sigma^{2}} \left(\frac{\nu\tau^{2} + ns^{2}}{\nu+n}\right)\right)$$

where $s^{2} = \frac{1}{n} \sum_{i=1}^{n} (y_{i} - z(\mathbf{x}_{i}))^{2}$.

Draw $\sigma^2 | \mathcal{T}, \mathcal{M}, \mathbf{y}$

• And we recognize $\frac{1}{\sigma^{(\nu+n)+2}} exp\left(-\frac{(\nu+n)}{2\sigma^2}\left(\frac{\nu\tau^2+ns^2}{\nu+n}\right)\right)$ as the kernel of a scaled-inverse-chisquared distribution, so

$$\sigma^2 | \mathcal{T}, \mathcal{M}, \mathbf{y} \sim \chi^{-2} \left(\nu + n, \frac{\nu \tau^2 + ns^2}{\nu + n} \right)$$

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• So we know how to perform the Gibbs step for σ^2 .

Draw $\mathcal{M}|\mathcal{T}, \sigma^2, \mathbf{y}$

• What about the terminal node scalar mean parameters?

Draw $\mathcal{M}|\mathcal{T}, \sigma^2, \mathbf{y}$

What about the terminal node scalar mean parameters?

1

Suppose there are B terminal nodes in tree T, η^b₁,..., η^b_b. It is important to note the following factorization of the likelihood:

$$\begin{aligned} (\sigma^2, \mathcal{T}, \mathcal{M} | \mathbf{y}) &\propto & exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^n \left(y_i - z(\mathbf{x}_i) \right)^2 \right) \\ &= & exp\left(-\frac{1}{2\sigma^2} \sum_{j=1}^B \sum_{i:y_i \in \eta_j^b}^{n_j} \left(y_i - \mu_j \right)^2 \right) \\ &= & \prod_{j=1}^B exp\left(-\frac{1}{2\sigma^2} \sum_{i:y_i \in \eta_j^b}^{n_j} \left(y_i - \mu_j \right)^2 \right) \end{aligned}$$

where n_j is the number of observations mapping to terminal nodes η_j^b and $\sum_j n_j = n$.



In other words, conditional on *T*, the scalar terminal node parameters are independent!

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- In other words, conditional on *T*, the scalar terminal node parameters are independent!
- So, we can simply write down the full conditional for each μ_j and draw them sequentially using Gibbs steps.

Draw $\mu_j | \mathcal{T}, \sigma^2, \mathbf{y}$

- Assuming mean-centered observations, our prior is

$$\pi(\mu_j|\mathcal{T}) = N(0, \sigma_{\mu}^2).$$

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 Based on our results from awhile ago (slides 9), the full conditional is

$$\pi(\mu_j | \sigma^2, \mathcal{T}, \mathbf{y}) \sim N\left(\left(\frac{n_j}{\sigma^2} + \frac{1}{\sigma_\mu^2}\right)^{-1} \left(\frac{n_j \overline{y}_j}{\sigma^2}\right), \left(\frac{n_j}{\sigma^2} + \frac{1}{\sigma_\mu^2}\right)^{-1}\right)$$

where $\bar{y}_j = \frac{1}{n_j} \sum_{i: y_i \in \eta_j^b} y_i$.

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- Chipman et al.[†] propose four basic proposals for mixing over tree-space: Birth, Death, Change and Swap.
 - We'll look at Birth and Death only for now.

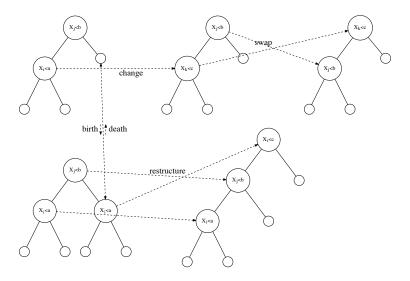


Figure 2: Tree Moves

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- This means that when we birth, a previous terminal node parameter μ disappears and two new parameters, say μ_(l) and μ_(r) are born.
- And when we death, two previous terminal node parameters, $\mu_{(l)}$ and $\mu_{(r)}$, dissappear and a new parameter μ is born.

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- Fortunately, Green (1995) shows that when the dimension-changing parameter can be marginalized out, one can proceed with the usual MH algorithm but using the marginalized likelihood.
- For our conjugate Normal prior on the μ's, this marginal likelihood is available.

Marginal Likelihood

- Marginalizing the portion of the likelihood associated with terminal node η_i^b , we have

$$L(\eta_j^b|\sigma^2, \mathbf{y}) = \int_{\mu_j} L(\eta_j^b|\mu_j, \sigma^2, \mathbf{y}) \pi(\mu_j) d\mu_j$$

(I will leave this as an excercise).

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- 3. Calculate

$$\alpha = \min\left\{1, \frac{\pi(\mathcal{T}'|\sigma^2, \mathbf{y})q(\mathcal{T}|\mathcal{T}')}{\pi(\mathcal{T}|\sigma^2, \mathbf{y})q(\mathcal{T}'|\mathcal{T})}\right\}$$

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Generate u ~ Uniform(0, 1). If u < α then accept T' otherwise reject.

• In Step 3, note that

$$\begin{aligned} \pi(\mathcal{T}'|\sigma^2, \mathbf{y}) &= L(\eta_{j(l)}^b|\sigma^2, \mathbf{y})L(\eta_{j(r)}^b|\sigma^2, \mathbf{y})\pi(\eta_j^b \text{is internal}) \\ &\times \pi(\eta_{j(l)}^b \text{is terminal})\pi(\eta_{j(r)}^b \text{is terminal}) \\ &\times \pi_v(v_j^b = v_b)\pi_c(c_j^b = c_b) \end{aligned}$$

and

$$egin{aligned} q(\mathcal{T}|\mathcal{T}') &= q(\mathcal{T}' o \mathcal{T}) &= \pi(ext{death proposal}) \ & imes \pi(ext{kill} \; \eta^b_{j(l)}, \eta^b_{j(r)} | ext{death proposal}) \ &= (1 - \pi_b) \pi_{d, \eta^b_j} \end{aligned}$$

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- And π_{d,η_j^b} is the probability of selecting node η_j^b to perform the death.
 - Usually this will be $\frac{1}{D'}$ where D' is the number of next-to-terminal-nodes in tree \mathcal{T}' .
 - An exception is when we have the root node as our tree (obviously we can't perform a death). In this case \(\pi_{d,\eta_{i}^{b}} = 0\).

Analogously, for Step 3 note that

$$\pi(\mathcal{T}|\sigma^2, \mathbf{y}) = L(\eta_j^b|\sigma^2, \mathbf{y})\pi(\eta_j^b \text{ is terminal})$$

and

$$\begin{array}{ll} q(\mathcal{T}'|\mathcal{T}) = q(\mathcal{T} \to \mathcal{T}') &= & \pi(\text{birth proposal}) \\ & \times \pi(\text{birth at } \eta_j^b | \text{birth proposal}) \\ & \times \pi_v(v_j^b = v_b) \pi_c(c_j^b = c_b) \\ &= & \pi_b \pi_{b,\eta_j^b} \pi_v(v_j^b = v_b) \pi_c(c_j^b = c_b) \end{array}$$

• Typically $\pi_{b,\eta_j^b} = \frac{1}{B}$ where B is the number of terminal nodes in tree \mathcal{T} .

- Typically $\pi_{b,\eta_j^b} = \frac{1}{B}$ where B is the number of terminal nodes in tree \mathcal{T} .
 - An exception is when, for example, there is no variable or cutpoint available to birth at η^b_j. In this case π_{b,η^b_i} = 0.

Death Proposals

• As you might imagine, it works similarly to Birth proposals.

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- I will spare you the details.

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- **3.** Draw $\sigma^2 | \mathcal{T}, \mathcal{M}, \mathbf{y}$
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$$\alpha(1-d)^{-\beta}$$

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- The variables are selected with a discrete uniform prior.
- The cutpoints are selected with a discrete uniform prior.
 - The number of cutpoints is hyperparameter we can choose. Default is numcuts = 100. This works well in general, sometimes we might like a more refined grid, say numcuts = 1,000.

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- The idea is that our data is unlikely all noise, so a conservative approach is to setup the prior such that it is very unlikely to estimate the variance to be greater than the sample variance of our data.
- The smaller ν the more concentrated on small σ the prior becomes.

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- In other words, this sets the prior up such that k standard deviations cover the range of the observed data.
- The greater is k, the more shrinkage a priori is applied to the mean parameters. The default is k = 2.

```
source("dace.sim.r")
```

```
# Generate response:
set.seed(88)
n=5; k=1; rhotrue=0.2; lambdatrue=1
design=as.matrix(runif(n))
l1=list(m1=outer(design[,1],design[,1],"-"))
l.dez=list(11=11)
R=rhogeodacecormat(l.dez,c(rhotrue))$R
L=t(chol(R))
u=rnorm(nrow(R))
z=L%*%u
  Our observed data:
```

```
y=as.vector(z)
```

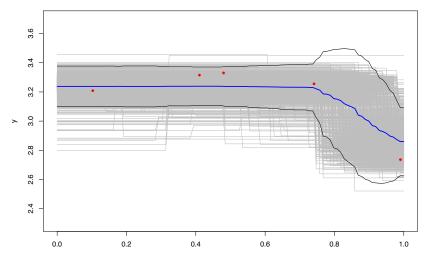
```
library(BayesTree)
preds=matrix(seq(0,1,length=100),ncol=1)
```

```
# Variance prior
shat=sd(y)
nu=3
q=0.90
# Mean prior
k=2
# Tree prior
alpha=0.95
beta=2
nc = 100
# MCMC settings
N=1000
burn=1000
```

```
##
##
## Running BART with numeric y
##
## number of trees: 1
## Prior.
   k: 2.000000
##
##
    degrees of freedom in sigma prior: 3
##
    quantile in sigma prior: 0.900000
    power and base for tree prior: 2.000000 0.950000
##
##
    use quantiles for rule cut points: 0
##
  data:
    number of training observations: 5
##
```

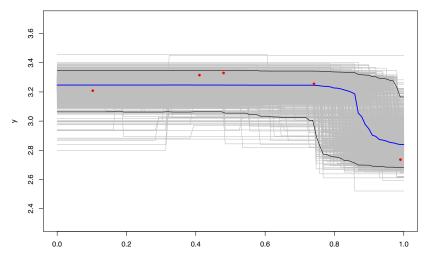
plot(design,y,pch=20,col="red",cex=2,xlim=c(0,1), ylim=c(2.3,3.7),xlab="x", main="Predicted mean response +/- 2s.d.") for(i in 1:nrow(fit\$yhat.test)) lines(preds,fit\$yhat.test[i,],col="grey",lwd=0.25) mean=apply(fit\$yhat.test,2,mean) sd=apply(fit\$yhat.test,2,sd) lines(preds,mean-1.96*sd,lwd=0.75,col="black") lines(preds,mean+1.96*sd,lwd=0.75,col="black") lines(preds,mean,lwd=2,col="blue") points(design,y,pch=20,col="red")

Predicted mean response +/- 2s.d.



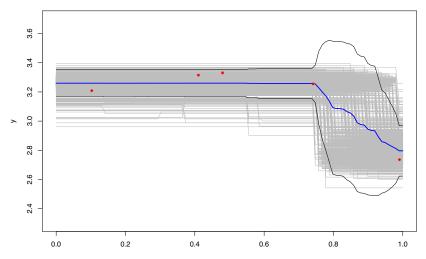
plot(design,y,pch=20,col="red",cex=2,xlim=c(0,1),ylim= xlab="x",main="Predicted median, q.025 and q.975") for(i in 1:nrow(fit\$yhat.test)) lines(preds,fit\$yhat.test[i,],col="grey",lwd=0.25) med=apply(fit\$yhat.test,2,quantile,0.5) q.025=apply(fit\$yhat.test,2,quantile,0.025) q.975=apply(fit\$yhat.test,2,quantile,0.975) lines(preds,q.025,lwd=0.75,col="black") lines(preds,q.975,lwd=0.75,col="black") lines(preds,med,lwd=2,col="blue") points(design,y,pch=20,col="red")

Predicted median, q.025 and q.975

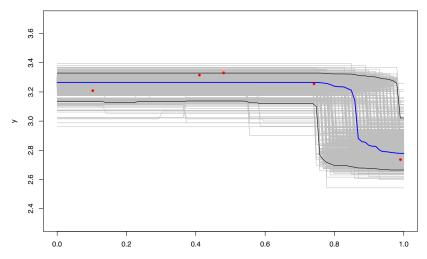


```
##
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## Running BART with numeric y
##
## number of trees: 1
## Prior.
## k: 2,000000
    degrees of freedom in sigma prior: 1
##
##
    quantile in sigma prior: 0.900000
##
    power and base for tree prior: 2.000000 0.950000
##
    use quantiles for rule cut points: 0
  data:
##
```

Predicted mean response +/- 2s.d.

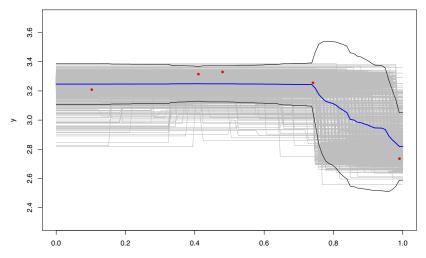


Predicted median, q.025 and q.975

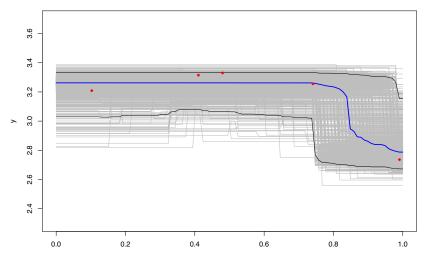



```
##
##
  Running BART with numeric y
##
##
## number of trees: 1
## Prior:
   k: 2.000000
##
    degrees of freedom in sigma prior: 1
##
##
    quantile in sigma prior: 0.900000
    power and base for tree prior: 2.000000 0.950000
##
##
    use quantiles for rule cut points: 0
```

Predicted mean response +/- 2s.d.



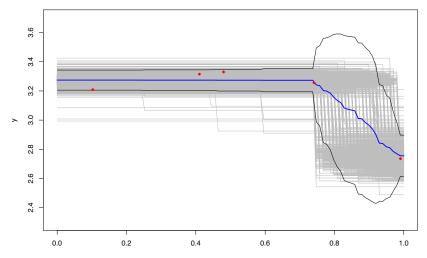
Predicted median, q.025 and q.975



nu=1
k=1
nc=100
<pre>fit=bart(design,y,preds,sigest=shat,sigdf=nu,sigquant=q,</pre>
<pre>k=k,power=beta,base=alpha,ntree=1,numcut=nc,</pre>
ndpost=N,nskip=burn)

```
##
##
##
Running BART with numeric y
##
## number of trees: 1
## Prior:
## k: 1.000000
## degrees of freedom in sigma prior: 1
## quantile in sigma prior: 0.900000
## power and base for tree prior: 2.000000 0.950000
```

Predicted mean response +/- 2s.d.





Predicted median, q.025 and q.975

