introduction to Bayesian state space models

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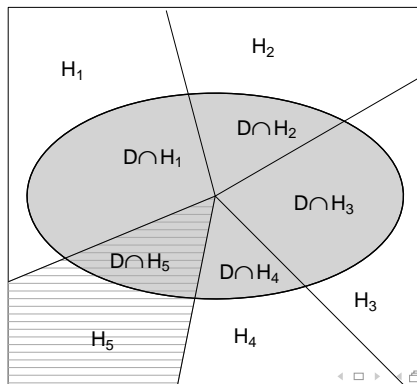
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Outline

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1. super-quick intro to Bayes

2. Markov chain Monte Carlo

3. State-space models

4. Other approaches to nonlinear dynamical fitting

Big picture

- use Bayes' rule
- avoid frequentist contortions
- integrate prior knowledge
- make coherent decisions
- compute hard things

Bayes rule

$$\underbrace{P(H_i|D)}_{\text{posterior}} = \underbrace{P(D|H_i)}_{\text{likelihood}} \underbrace{P(H_i)}_{\text{prior}} / \underbrace{\sum_j P(H_j)P(D|H_j)}_{P(\text{data})}$$

priors: $P(H_i)$

- usually framed as "prior belief"

- controversial because subjective

- if we set all $P(H_i)$ equal, $P(H_i|D) = P(D|H_i)/\sum P(D|H_j)$ (**scaled likelihood**)

- can't really be swept under the rug

more on priors

- **weak** or **diffuse**: little information
- **uninformative** or **flat**: no information
- **improper**: integral diverges (but sometimes OK)
- weak priors can cause problems with sparse data and/or weakly identifiable models
- **conjugate** priors: convenient functional forms

effects of priors
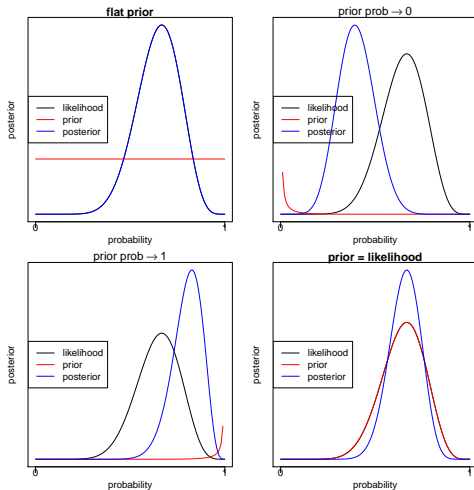
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Markov chain Monte Carlo

- **general** method for sampling posterior probability densities
- construct a Markov chain whose stationary density equals the desired posterior probability density
- avoids computation of Bayes' rule denominator ($\iint P(\boldsymbol{\theta}) \, d\boldsymbol{\theta}$)

you won't believe these two MCMC tricks

Gibbs sampling   sample parameters one at a time,
exploiting conditioning

Rejection sampling   (Metropolis-Hastings): pick new values of
parameters at random, then pick a random number to
decide whether to keep them

Gibbs sampling

Because $\mathrm{Prob}(A|B) = \mathrm{Prob}(A, B)/\mathrm{Prob}(B)$, we can say

$\mathsf{Prob}(A, B, C, \ldots Z) \propto \mathsf{Prob}(A|B, \ldots, Z) \cdot \mathsf{Prob}(B|C, \ldots, Z) \cdot \ldots \mathrm{Prob}(Z)$

This means that we can sample the conditional probabilities
sequentially and get the right answer.
picture of sampling

Metropolis-Hastings

Jump, evaluate (prior $\times$ likelihood), decide whether to accept

$$\frac{\text{Prob}(A)}{\text{Prob}(B)} = \frac{P(\text{jump } B \to A) \cdot P(\text{accept } A|B)}{P(\text{jump } A \to B) \cdot P(\text{accept } B|A)}$$

In the long run our chain will converge to the right distribution

- **candidate distribution**: anything sensible
  (bad choices make sampling slow, but not incorrect)

- **acceptance rule**:

$$P(\text{accept } \theta_2) = \max\left(1, \frac{\Pr(\theta_2)L(\theta_2)}{\Pr(\theta_1)L(\theta_1)}\right)$$

  i.e. "always accept if θ_2 better: sometimes if θ_2 worse"

Magic black boxes

- Can construct your own, customized samplers (Bolker et al., 2003)
- Use BUGS (Bayesian Inference Using Gibbs Sampling) language (`WinBUGS`, `OpenBUGS`, `JAGS`, `NIMBLE`)
- interfaces from R (`R2jags package`) or MATLAB (https://github.com/msteyvers/matjags).

Outline

State space models

- address fundamental problem: prob(observations) depends on **unobserved** true values
- have to deal with/integrate over all possible values (**latent variables**)
- very high-dimensional: brute force fails
- use the previous two tricks

important: often need to handle obs+proc error in some way to get reliable answers and CIs (King et al., 2015)

BUGS code for the logistic function

```
model <- function() {
  t[1] <- n0     ## initial values ...
  o[1] ~ dnorm(t[1],tau.obs)
  for (i in 2:N) {   ## step through observations ...
     v[i] <- t[i-1]+r*t[i-1]*(1-t[i-1]/K)
     t[i] ~ dnorm(v[i],tau.proc)
     o[i] ~ dnorm(t[i],tau.obs)
  }
  r ~ dunif(0.1,maxr) ## priors ...
  ## rate and scale of gamma
  K ~ dgamma(0.005,0.005)
  tau.obs ~ dgamma(0.005,0.005)
  tau.proc ~ dgamma(0.005,0.005)
  n0 ~ dgamma(1,n0rate)
}
```

Dependency structure for logistic model
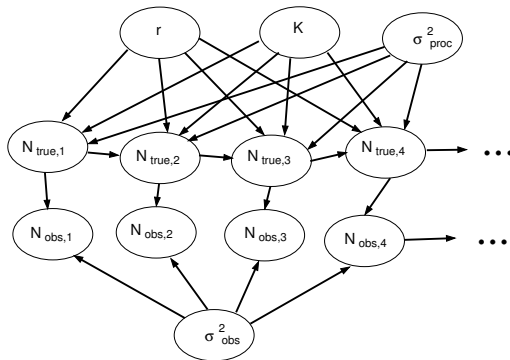
BUGS vs R

- BUGS code is not sequential (!)
- BUGS is not vectorized (need `for` loops)
- BUGS: ~ means "distributed as" ("stochastic node")
  <- means assignment ("logical node")
- different distribution names and parameterizations (e.g. `dnorm(mean,prec)` for Normal, `dbin(size,prob)` for binomial): see LeBauer et al. (2013)

Running JAGS

- **Good news**: JAGS code is (relatively) intuitive
- **Bad news**:
  - Debugging is hard
  - Need to figure out how long to run chains (convergence diagnostics)
  - Poor mixing
  - Slow computation

Running JAGS (details)

- specify model and priors
- get model to compile
- run multiple chains
  - discard **burn-in**
  - thin results
- assess convergence

Troubleshooting JAGS

- simplify model
- specify initial values explicitly
- narrow priors and/or fix some parameters
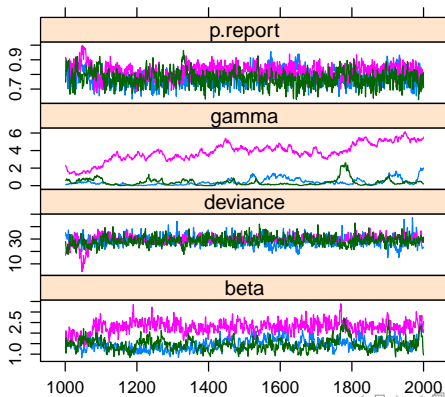- run longer and thin more

Speeding up MCMC

- reparameterize
- try Hamiltonian MC (Carpenter et al., 2016)
- block (correlated) updates to some parameters
- narrow priors and/or fix some parameters

Diagnostics example

trace plots: should look like white noise

```
library(R2jags); library(coda); library(lattice)
xyplot(as.mcmc(jagsout))
```
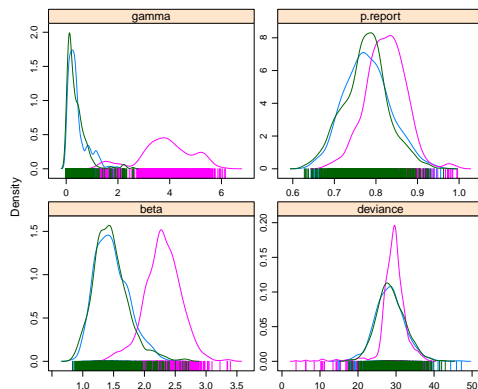
Diagnostics example

Gelman-Rubin statistic: want $\hat{R} < 1.2$

```
gelman.diag(as.mcmc(jagsout))

## Potential scale reduction factors:
##
##          Point est. Upper C.I.
## beta           2.69       4.78
## deviance       1.01       1.04
## gamma          4.48      13.58
## p.report       1.19       1.54
##
## Multivariate psrf
##
## 3.49
```

Also look at **effective sample size**, `n.eff` in some output
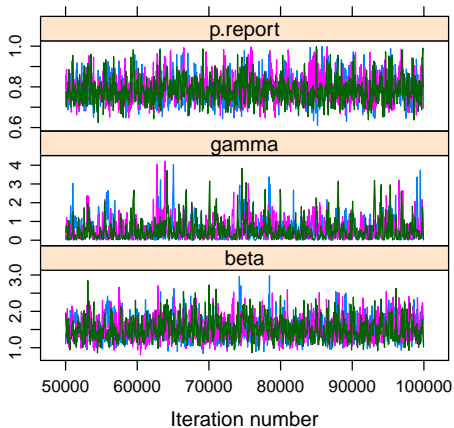
Density plots

Summary example

```
summary(as.mcmc(jagsout))
```

```
##                Mean      SD Naive SE Time-series SE
## beta         1.7420 0.48411 0.008839       0.023546
## deviance    28.8052 3.73637 0.068217       0.232341
## gamma        1.5430 1.75101 0.031969       0.164691
## p.report     0.7929 0.05669 0.001035       0.003175
```

run for 10^5 steps . . .

summary, 10^5 steps

```
## Inference for Bugs model at "sir.jags", fit using jags,
##  3 chains, each with 1e+05 iterations (first 50000 discar
##  n.sims = 3000 iterations saved
##            mean   sd 2.5%  25%  50%  75% 97.5% Rhat n.eff
## beta       1.52 0.32 1.03 1.29 1.46 1.70  2.26    1  3000
## gamma      0.54 0.56 0.02 0.16 0.37 0.74  2.09    1  3000
## p.report   0.79 0.06 0.68 0.75 0.78 0.82  0.94    1  1800
##
## For each parameter, n.eff is a crude measure of effective
## and Rhat is the potential scale reduction factor (at conv
```

Inference from posteriors

- point estimates: mean, median (marginal)
- interval estimates: quantiles, **highest posterior density** (`coda::HPDinterval`)
- can summarize any quantity computed from samples (e.g. predictions)

Further resources

- Gelman et al. (2013) (fairly hard-core)
- Gelman and Hill (2006) (more regression-focused)
- Hobbs and Hooten (2015) (friendlier, ecologist-focused)
- McCarthy (2007) (even friendlier)

The problem with MCMC (xkcd)
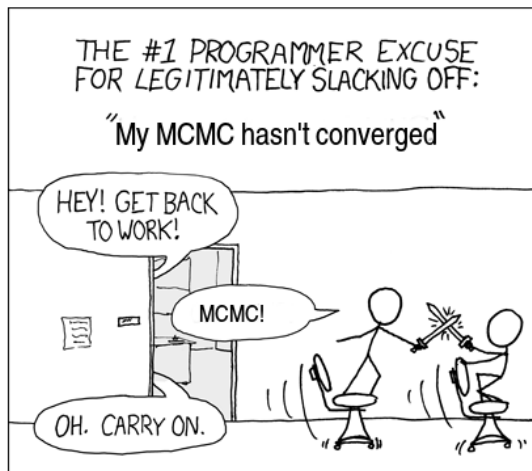
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advances in MCMC

- new toolboxes: NIMBLE (Li et al., 2017; de Valpine et al., 2017), PyMC
- Hamiltonian Monte Carlo: Stan (Carpenter et al., 2016)
- variational Bayes, expectation-propagation . . . (Gelman et al., 2013)

Frequentist alternatives

- MCMC is usually Bayesian;
  opens various cans of worms
- there are many other related approaches, some classical
    - expectation-maximization
    - sequential Monte Carlo/particle filters (Ionides et al., 2006;
      Doucet et al., 2001; de Valpine, 2004): R pomp, NIMBLE
      packages, PyMC
    - data cloning (Lele et al., 2007): R dclone package

Estimation for continuous-time models

Particle methods (freq or Bayesian)

- simulate many trajectories ("particles") step-by-step
- at each step, resample particles weighted by likelihood of current location

Approximate Bayesian computation

- sample parameters from prior
- simulate trajectories for each parameter set
- compute summary statistics ("probes")
- save trajectories with summary stats near observed values

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