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Beyond Metropolis Sampling: Gibbs & Hamiltonian Sampling

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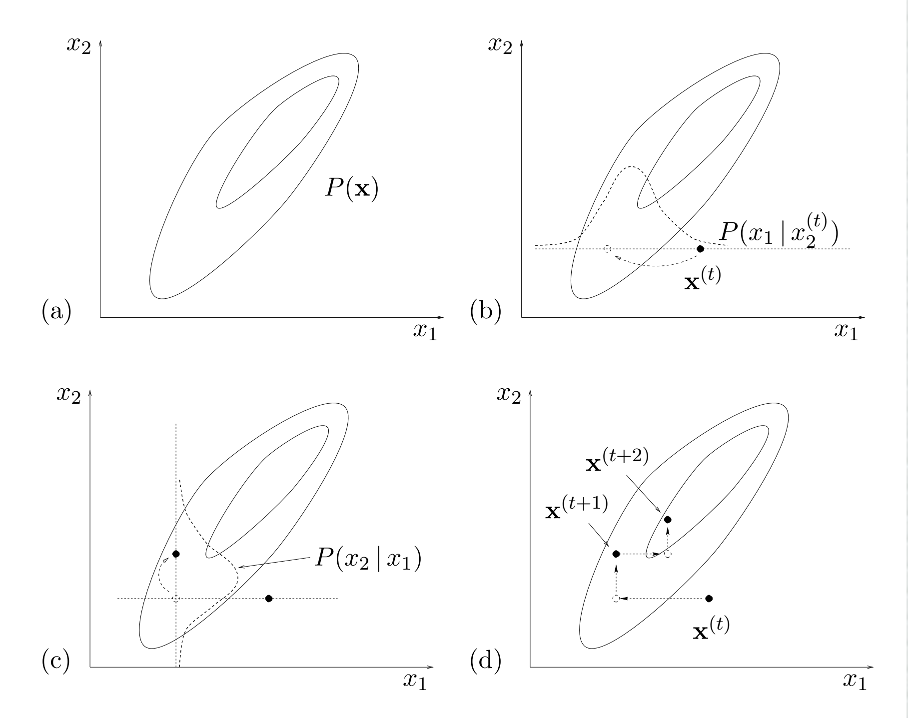
Sampling beyond MCMC

- Simple MCMC is a good general tool, but
  - curse of dimensionality
  - requires tuning — e.g., proposal distributions
  - inefficient
- Other sampling techniques exist
  - usually for cases when you have more information about the distributions
  - Gibbs sampling — need to have the conditional probabilities for different parameters, $P(\theta_1|\theta_2,d)$
  - Hamiltonian Monte Carlo — need derivatives $\partial P(\theta)/\partial\theta$

Gibbs Sampling



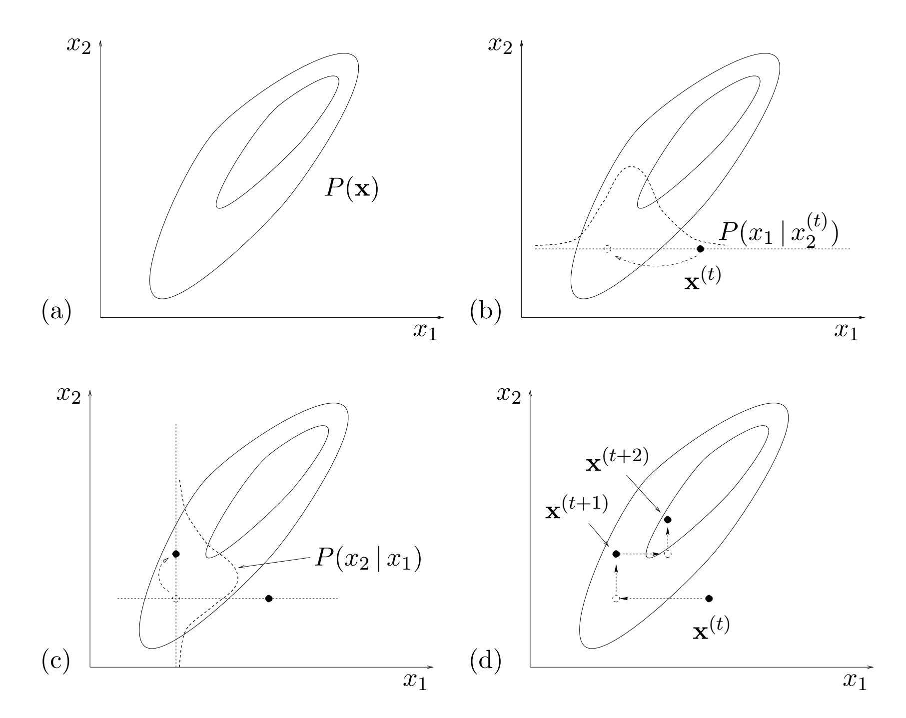
McKay, *Information Theory…*

- Metropolis-Hastings with Proposal = conditional dist'n
  - all samples accepted
  - satisfies detailed balance
  - no adjustable parameters in the algorithm
- suited to hierarchical models (often written in terms of the conditionals)
- Algorithm:
  - $x_1^{(n+1)} \sim P(x_1|x_2^{(n)}, x_3^{(n)},\ldots)$
    $x_2^{(n+1)} \sim P(x_2|x_1^{(n+1)}, x_3^{(n)},\ldots)$
    $x_3^{(n+1)} \sim P(x_3|x_1^{(n+1)}, x_2^{(n+1)},\ldots)$
  - Should change (reverse/randomize) the order 1, 2, 3,… in successive steps
- Caveats: can fail badly if the distribution isn't aligned with the axes and/or highly curved
- *Otherwise often use "metropolis-within-Gibbs"

Especially good if these can be "analytically" sampled*

Gibbs Sampling

- Algorithm:
  - $x_1^{(n+1)} \sim \mathrm{P}(x_1 | x_2^{(n)}, x_3^{(n)}, \ldots)$
    $x_2^{(n+1)} \sim \mathrm{P}(x_2 | x_1^{(n+1)}, x_3^{(n)}, \ldots)$
    $x_3^{(n+1)} \sim \mathrm{P}(x_3 | x_1^{(n+1)}, x_2^{(n+1)}, \ldots)$



McKay, *Information Theory…*

- Note that conditional distributions are just the full distribution with the other parameters held fixed (up to normalization).

$$P(x \mid y) = \frac{P(x, y)}{P(y)} \propto P(x, y)$$

- In a hierarchical model, get the full posterior by multiplying out all the distributions that appear
  - See Alan Heavens' talk later…

Hamiltonian Monte Carlo (HMC)

- *(aka Hybrid Monte Carlo; Duane et al 1987)*
- Analogy with dynamical systems, which explore (***position, momentum***) phase space over time
  - Potential $U(\theta_i) = -\ln \mathrm{P}(\theta_i)$ w/ "positions" θ_i
  - KE $K(u_i) = \frac{1}{2}\boldsymbol{u}\cdot\boldsymbol{u}$ w/ "momenta" $u_i \sim \mathrm{N}(0,\sigma^2)$
  - Hamiltonian $H(\theta_i, u_i) = U(\theta_i) + K(u_i)$
  - Density $\mathrm{P}(\theta_i, u_i) = e^{-H(\theta, u)}$
    - 2N parameters!
  - Evolve as dynamical system
    - ignore (marginalize over) momenta

$$\dot{\theta}_i = \frac{\partial H}{\partial u_i} = u_i$$

$$\dot{u}_i = -\frac{\partial H}{\partial \theta_i} = \frac{\partial \ln P}{\partial \theta_i}$$

- Need to discretize the system (time derivatives)
- Values of (θ_i, u_i) at different times: proposed MC samples
- If exact dynamics, H conserved, $\Longrightarrow$ all samples accepted
  - in practice, approximate evolution (and, e.g., numerical derivatives)
  - so, accept $(\theta_i, u_i)^*$ as step $n+1$ with probability

$$\min\left[1, \exp\left(-H^* + H^{(n)}\right)\right]$$

$$\dot{\theta}_i = \frac{\partial H}{\partial u_i} = u_i$$

$$\dot{u}_i = -\frac{\partial H}{\partial \theta_i} = \frac{\partial \ln P}{\partial \theta_i}$$

HMC Algorithm (1)

- Algorithm (Hajian *PRD*75 083525, 2007)

```
initialize x_(0)
for i = 1 to N_samples
    u ~ N(0, 1)
    (x*_(0), u*_(0)) = (x_(i-1), u)
    for j = 1 to N
        make a leapfrog move: (x*_(j-1), u*_(j-1)) → (x*_(j), u*_(j))
    end for
    (x*, u*) = (x_(N), u_(N))
    draw α ~ Uniform(0, 1)
    if α < min{1, e^{-(H(x*,u*) - H(x,u))}}
        x_(i) = x*
    else
        x_(i) = x_(i-1)
end for
```

Only propose every N timesteps

Discretisation step!
(see problem sheet)

HMC Algorithm (2)

- R version (Neal, in *Handbook of MCMC*)

```
HMC = function (U, grad_U, epsilon, L, current_q)
{
  q = current_q
  p = rnorm(length(q),0,1)  # independent standard normal variates
  current_p = p

  # Make a half step for momentum at the beginning
  p = p - epsilon * grad_U(q) / 2

  # Alternate full steps for position and momentum

  for (i in 1:L)
  {
    # Make a full step for the position
    q = q + epsilon * p
    # Make a full step for the momentum, except at end of trajectory
    if (i!=L) p = p - epsilon * grad_U(q)
  }

  # Make a half step for momentum at the end.
  p = p - epsilon * grad_U(q) / 2
  # Negate momentum at end of trajectory to make the proposal symmetric
  p = -p

  # Evaluate potential and kinetic energies at start and end of trajectory

  current_U = U(current_q)
  current_K = sum(current_p^2) / 2
  proposed_U = U(q)
  proposed_K = sum(p^2) / 2

  # Accept or reject the state at end of trajectory, returning either
  # the position at the end of the trajectory or the initial position

  if (runif(1) < exp(current_U-proposed_U+current_K-proposed_K))
  {
    return (q)  # accept
  }
  else
  {
    return (current_q)  # reject
  }
}
```

Single L-step trajectory

Leapfrog method

HMC vs Metropolis-Hastings

Two trajectories

Four trajectories

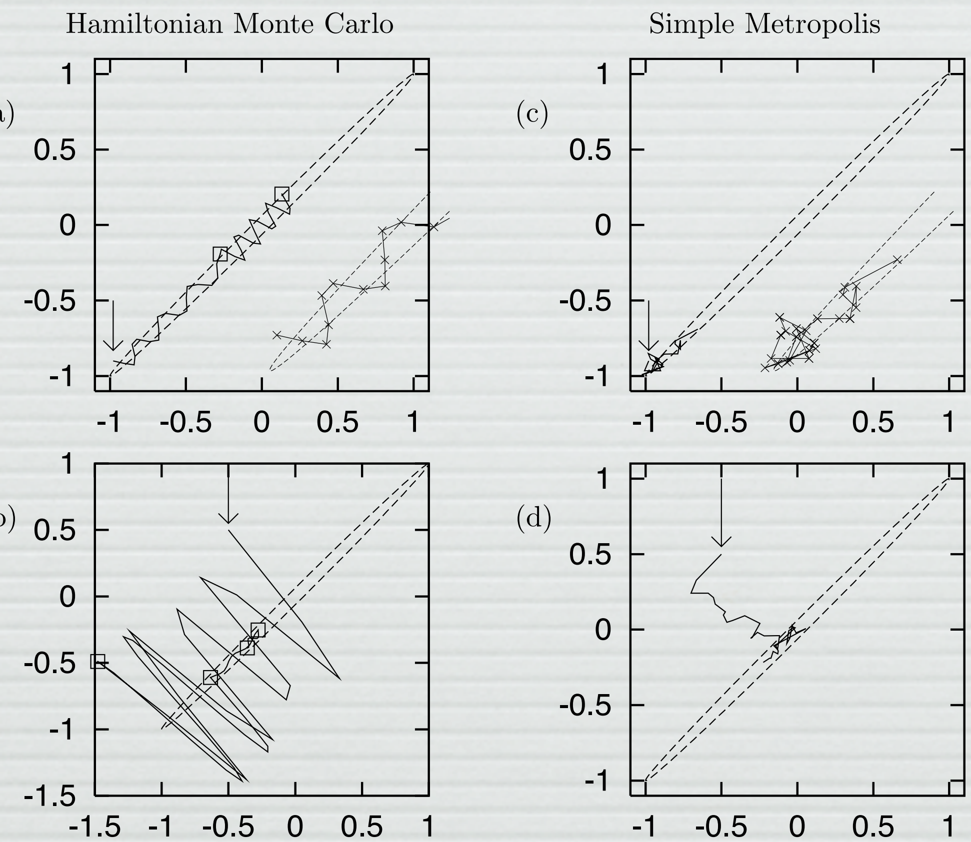


Figure 30.2. (a,b) Hamiltonian Monte Carlo used to generate samples from a bivariate Gaussian with correlation $\rho = 0.998$. (c,d) For comparison, a simple random-walk Metropolis method, given equal computer time.

MacKay, *Information Theory…*

Neil, *Handbook of MCMC*

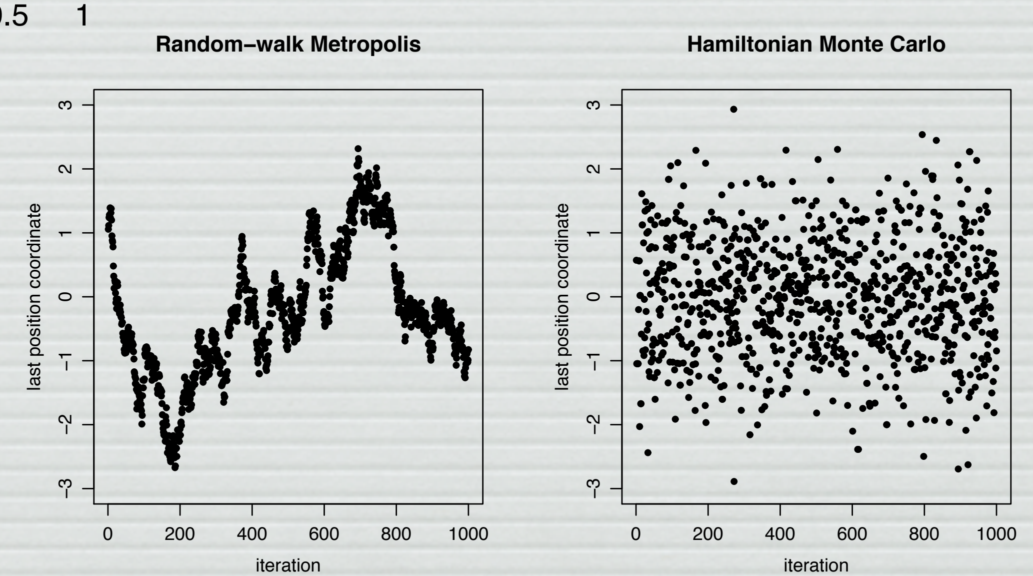
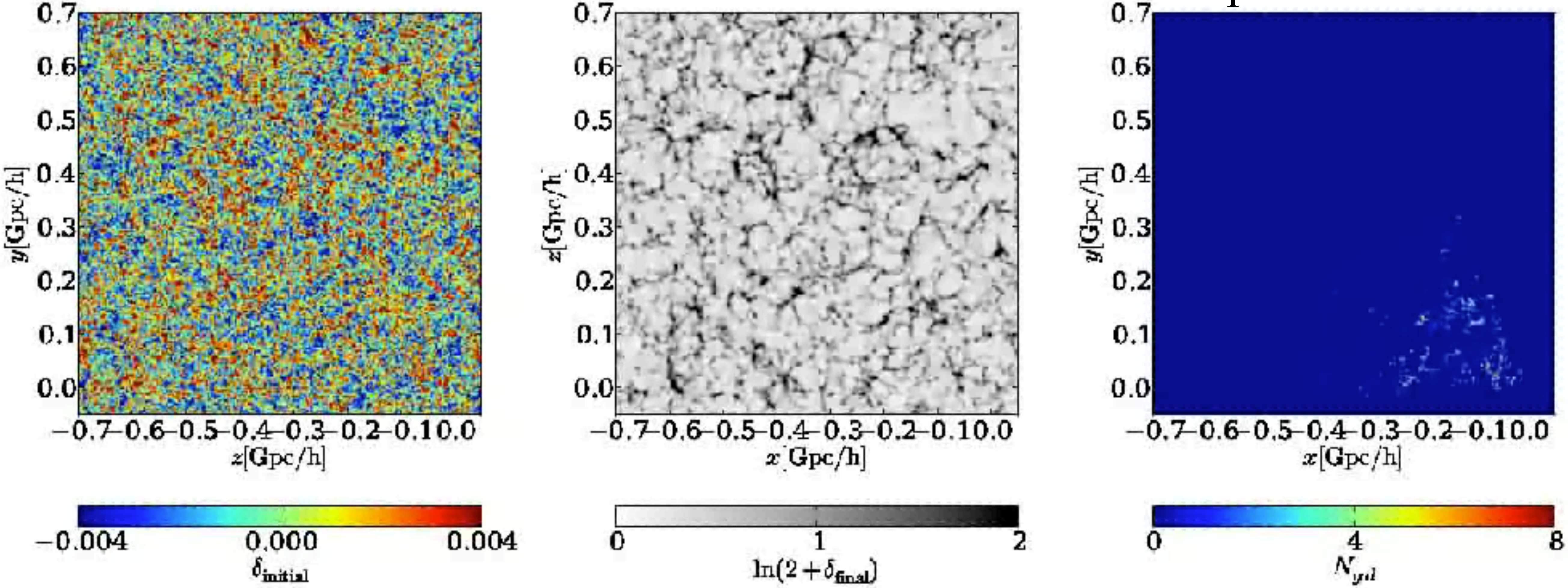


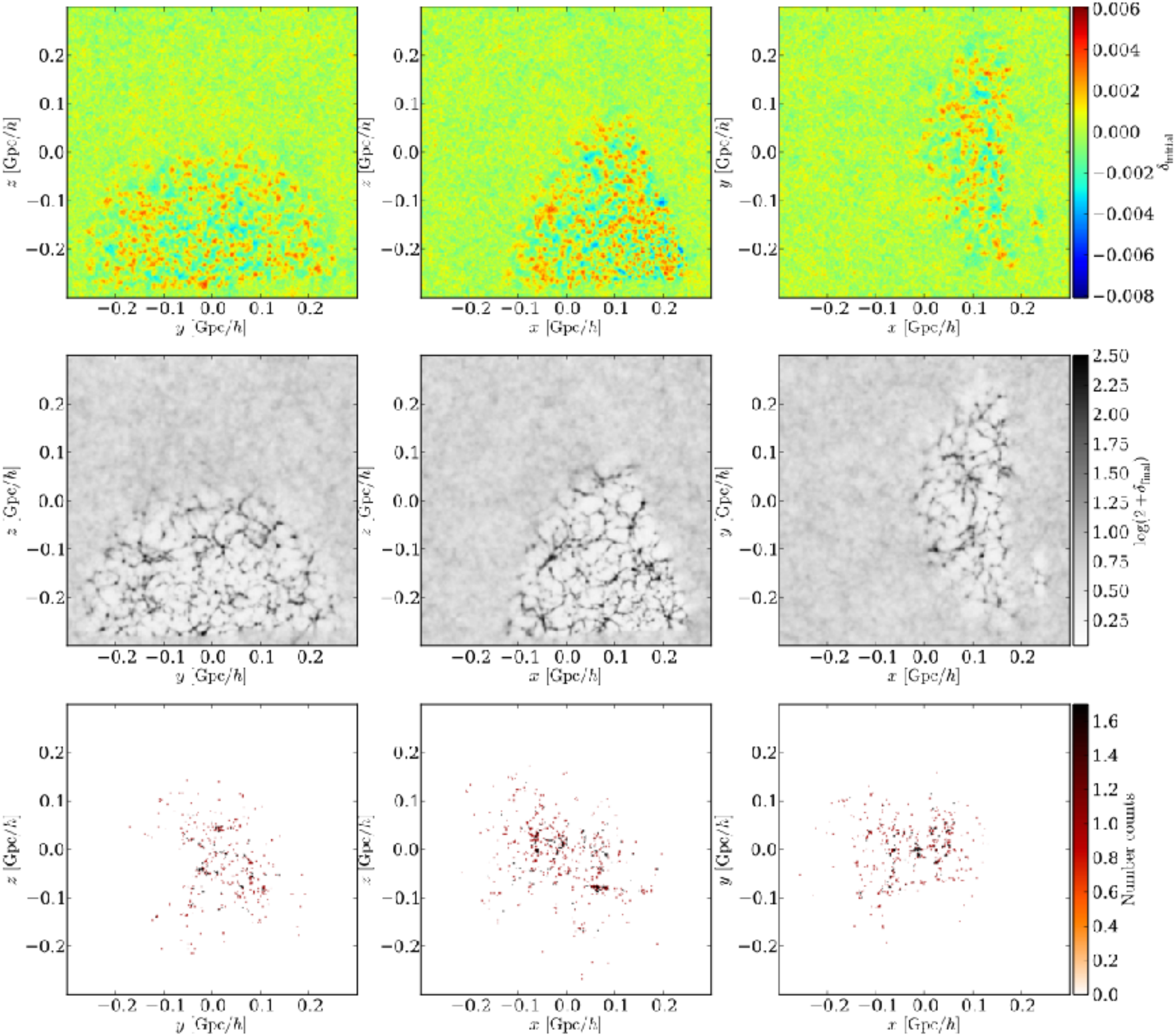
Figure 6: Values for the variable with largest standard deviation for the 100-dimensional example, from a random-walk Metropolis run and an HMC run with $L = 150$. To match computation time, 150 updates were counted as one iteration for random-walk Metropolis.

HMC with millions of parameters

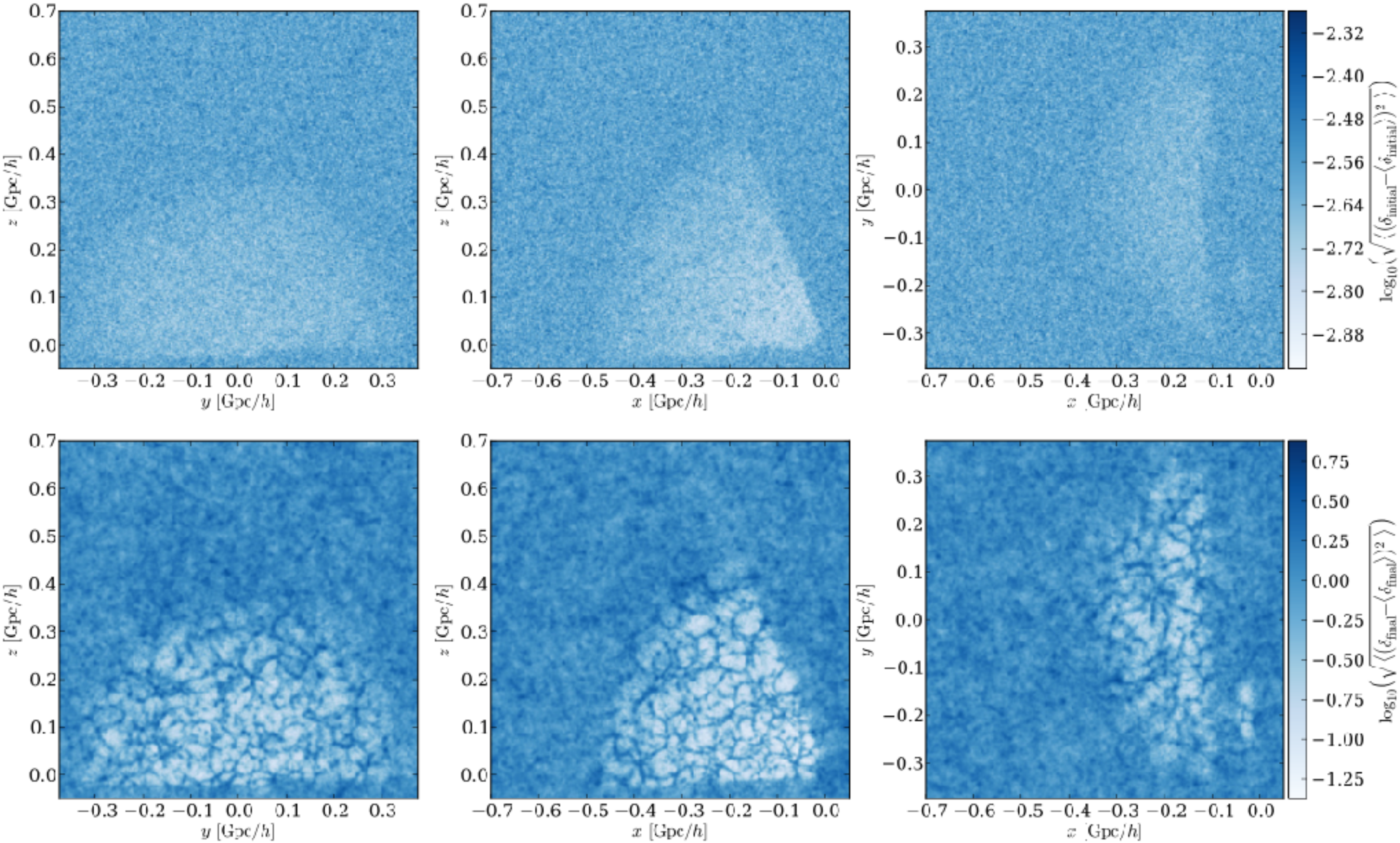
- From large-scale structure observations to the *primordial* density field
  - forward physics model from primordial density to observed galaxy distribution
- Related work from Jasche, Lavaux,, Kitaura

F. Leclercq & B.Wandelt





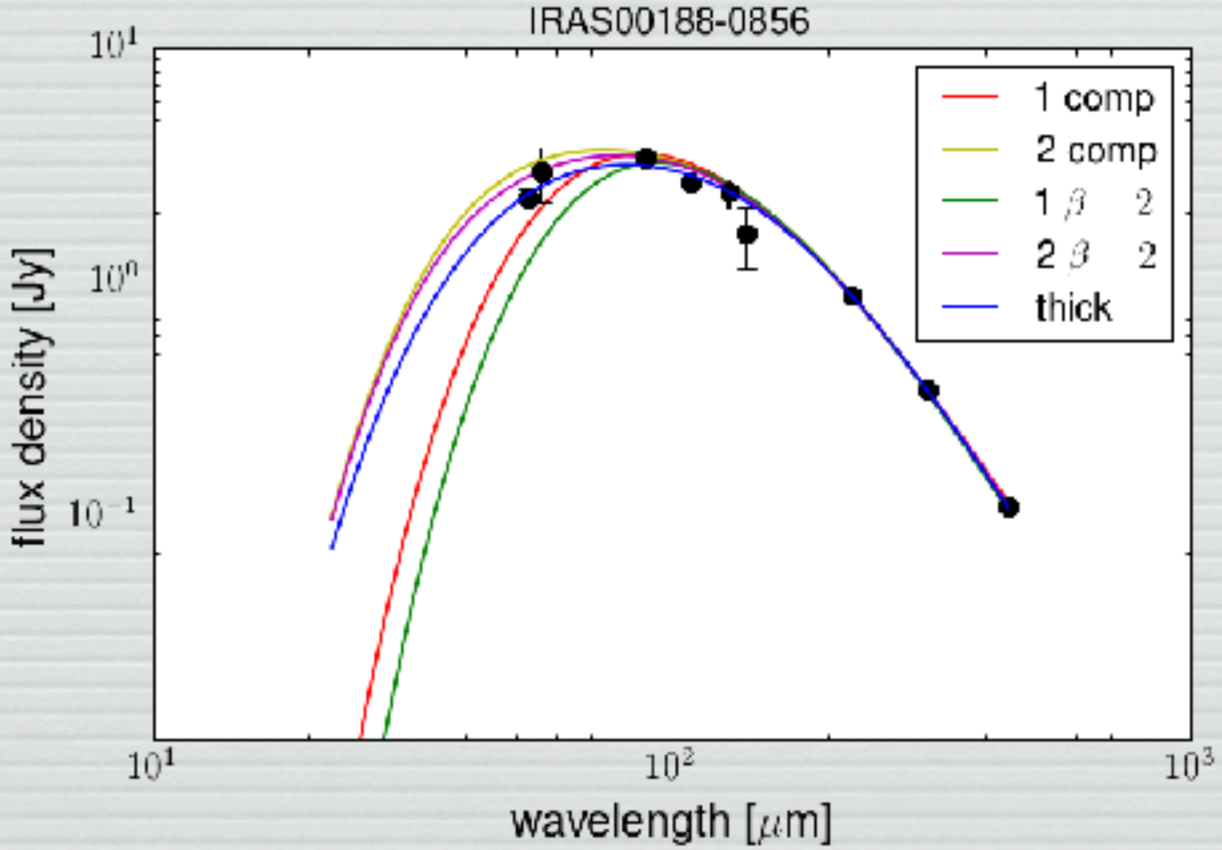
z [Gpc/h]
y [Gpc/h]
x [Gpc/h]
$\delta_{\rm initial}$
$\log(2+\delta_{\rm final})$
Number counts

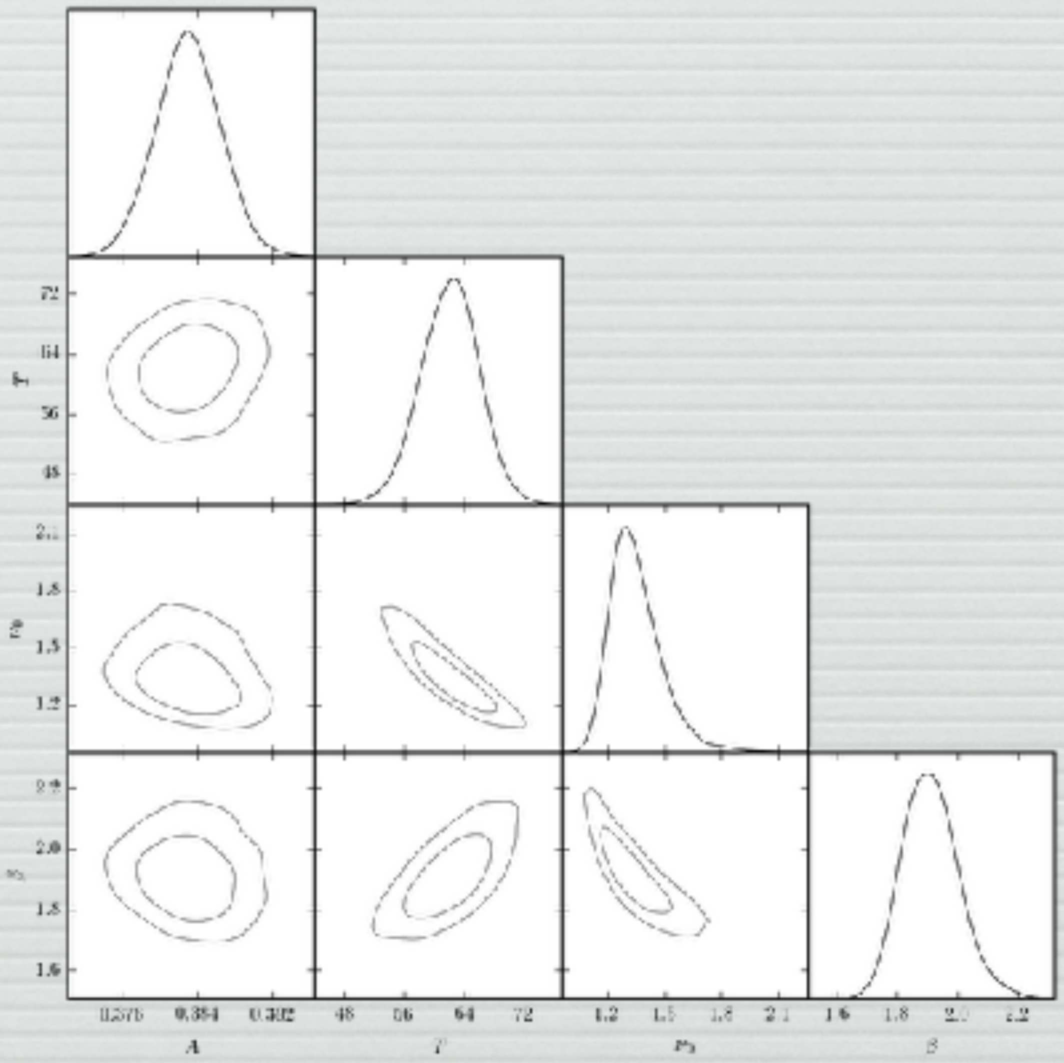


z [Gpc/h]
y [Gpc/h]
x [Gpc/h]
z [Gpc/h]
y [Gpc/h]
$\log_{10}\left(\sqrt{\langle(\delta_{\mathrm{initial}}-\langle\delta_{\mathrm{initial}}\rangle)^2\rangle}\right)$
$\log_{10}\left(\sqrt{\langle(\delta_{\mathrm{final}}-\langle\delta_{\mathrm{final}}\rangle)^2\rangle}\right)$

HMC as a generic tool

- Gelman et al, STAN (http://mc-stan.org/)
- Uses *automatic differentiation* to get derivatives for ~anything that can be built up from elementary functions
- e.g., SED fitting





Stan Code

```
data {

    int<lower=1> N_comp;   // # of greybody components
                           // (fixed model parameter)

    int<lower=1> N_band;   // number of photometric bands
    vector[N_band] nu_obs; // observed frequency
    vector[N_band] flux;   // observed flux
    vector[N_band] sigma;  // error
    real z;                // redshift

}


transformed data {

    vector[N_band] nu;     // rest frame frequency
    nu = (1+z)*nu_obs;

}


functions {

    real greybody(real beta, real T, real nu) {
      // greybody, normalized to unit flux at nu=nu_0
        real h_over_k;
        real x;
        real nu_bar;
        real x_bar;

        nu_bar = 1000;

        h_over_k = 0.04799237;       //  K/Ghz
        x = h_over_k * nu / T;
        x_bar = h_over_k * nu_bar / T;
        return (pow(nu/nu_bar, 3+beta) *
               expm1(x_bar) / expm1(x));
    }

}
```

```
parameters {

// nb. N_comp, N_band are data
   vector<lower=0>[N_comp] amplitude;
   positive_ordered[N_comp] T;

// greybody factor
   vector<lower=0, upper=3>[N_comp] beta;

}

model {

    real fluxes[N_band, N_comp];
    vector[N_band] totalflux;

    for (band in 1:N_band) {
        for (comp in 1:N_comp) {  // vectorize over this?
            fluxes[band, comp] = amplitude[comp] *
              greybody(beta[comp], T[comp], nu[band]);
        }
        totalflux[band] = sum(fluxes[band]);
    }

    // try a proper prior on temperature;
    //    needed since ordered vectors don't have limits
    T ~ uniform(3,100);
    flux ~ normal(totalflux, sigma);

}
```

Inference from a Gaussian: Averaging

- The simplest "linear model"
- Consider *data* = *signal* + *noise*,
- $d_i = \mu + n_i$ for data points $i=1\ldots N$
  - Noise, n_i, has zero mean, known variance σ^2
    - Assign a Gaussian to $(d_i - \mu)$
      - Alternately: keep n_i as a parameter and marginalize over it with $p(d_i|n_i \mu I) = \delta(d_i - n_i - \mu)$
  - Prior for s (*i.e.*, a and b)?
    - To be careful of limits, could use Gaussian with width Σ, take $\Sigma\rightarrow\infty$ at end of calculation
      - Same answer with unifom dist'n in $(-\Sigma_1,\Sigma_2)\rightarrow(-\infty,\infty)$

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→calculation

Inference from a Gaussian: Averaging

- Posterior:

$$P(\mu\,|\,d) = \frac{1}{\sqrt{2\pi\sigma_b^2}} \exp\left[-\frac{1}{2}\frac{(\mu-\bar{d})^2}{\sigma_b^2}\right]$$

  - best estimate of signal is average ± stdev:
    - $\mu = \bar{d} \pm \sigma_b = \bar{d} \pm \sigma/\sqrt{N}$
  - What if we don't know σ? try Jefferys $P(\sigma|I) \propto 1/\sigma$
    - marginalize over μ: $P(\mu\,|\,d) \propto \left[\mu^2 - 2\mu\bar{d} + \bar{d}^2\right]^{-1/2}$
      - Student t or Cauchy distribution
        - (very broad distribution!)

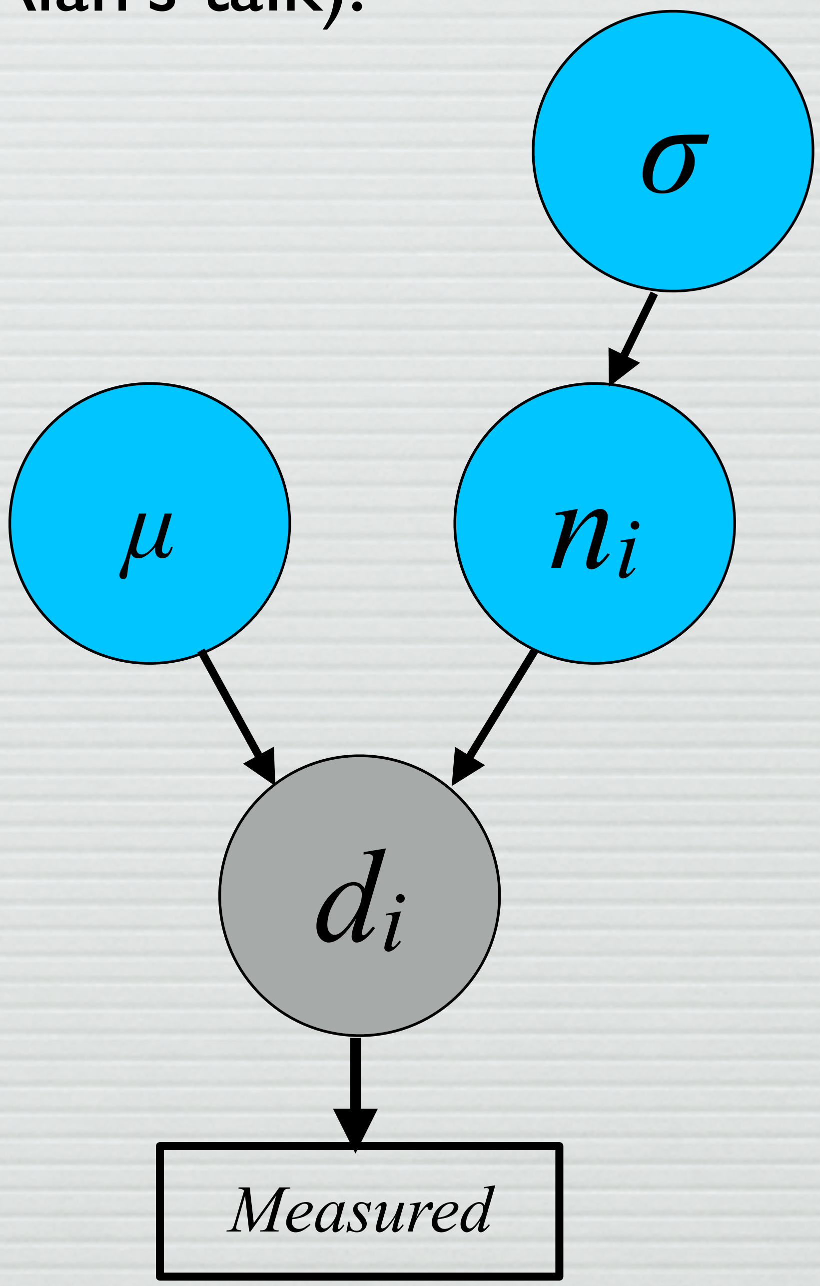
A toy model: estimating the mean and variance

- Back to our averaging problem, $d_i = s + n_i$
- $P(n_i|I)$ = Gaussian w/ $\langle n_i \rangle = 0$, $\langle n^2 \rangle = \sigma^2$
- $P(s|I)$ = Uniform
- Toy version of measuring cosmological maps and power spectra (see Alan Heaven's talk)

- Take σ^2 ***unknown*** w/ prior

  $P(\sigma) \propto 1/\sigma$ (improper…)

- Hierarchical model (see Alan's talk):

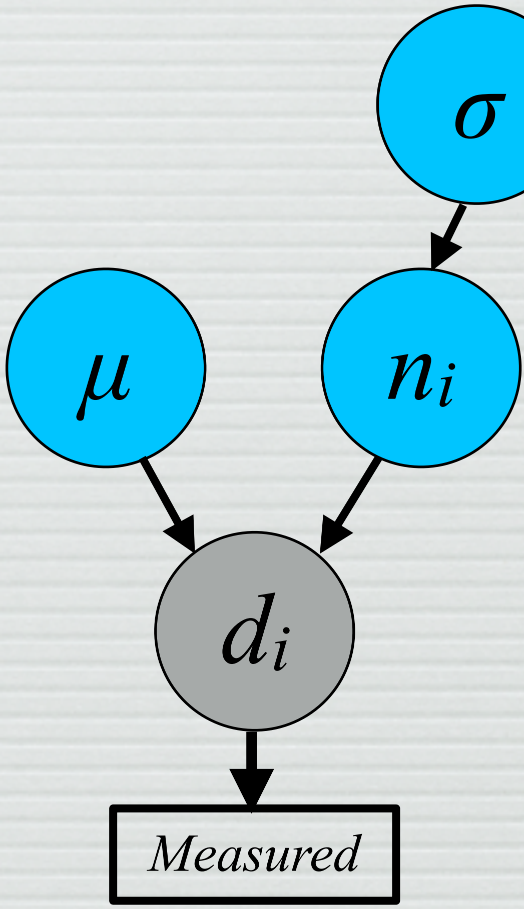


A toy model: estimating the mean and variance

- Back to our averaging problem, $d_i = \mu + n_i$

$$P(\mu,\sigma|d) = \frac{1}{\sigma}\frac{1}{(2\pi\sigma^2)^{n/2}}\exp\left[-\frac{n}{2\sigma^2}\left(\bar{d^2} - 2\mu\bar{d} + \mu^2\right)\right]$$

$$\propto \frac{1}{\sigma^{n+1}}\exp\left[-\frac{1}{2}\frac{\left(\mu-\bar{d}\right)^2}{\sigma^2/n}\right]\exp\left[-\frac{n}{2\sigma^2}\left(\bar{d^2} - \bar{d}^2\right)\right]$$



  - Unknown noise variance σ^2, Uniform prior on μ
  - Posterior is Gaussian in μ, Gamma in $1/\sigma^2$
  - Conditionals are known for Gibbs.

- Algorithm:

$$\mu|(\sigma^2, d) \leftarrow \text{Normal}\left(\bar{d}, \sigma^2/n\right)$$

$$\sigma^2|(\mu, d) \leftarrow \text{InvGamma}\left(\frac{n-1}{2}, \frac{n}{2}\left[\bar{d^2} - 2\mu\bar{d} + \mu^2\right]\right)$$

Case study

- Estimating a mean and variance.

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