Look Ma, No Sampling!

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Tired of waiting for your MCMC to run? No problem, just skip the MCMC and evaluate expectations using tensor train function representation and numerical integration.

Bayesian Formulation

θ Hyperparameters: Hyper-prior: $[\theta]$

x Latent field: Representation and prior $[x|\theta]$

y Observed data: Likelihood: $[y|x]$

Posterior Inference

The focus of inference is the posterior distribution:

try blblbl

$$[x,\theta|y] = \frac{[y|x]\,[x|\theta]\,[\theta]}{[y]}$$

We assume the normalizing constant $[y]$ is finite.
We wish to compute expectations:

$$\mathrm{E}_{x,\theta|y}[f(x)] = \int f(x)[x,\theta|y]\,\mathrm{d}x\,\mathrm{d}\theta$$

This Notation

We learned this notation from Alan Gelfand:
Read $[a]$ as "the distribution over a", and $[a|b]$ as "the distribution over a given b". We will abuse this notation to also denote the density function.

DO THIS

Quadrature and the Law of Total Expectation

The posterior expectation of any function $h(x)$ may be written

$$\mathrm{E}_{x,\theta|y}[h(x)] = \mathrm{E}_{\theta|y}\left[\mathrm{E}_{x|\theta,y}[h(x)]\right]$$

We compute the outer expectation by quadrature (see next panel). When the inner expectation is cheap to calculate, evaluating $\mathrm{E}_{x,\theta|y}[h]$ requires **no MCMC**.

DON'T DO THIS

Monte Carlo Integration

$$\mathrm{E}_{x,\theta|y}[f(x)] \approx \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

where $\{(x_i,\theta_i)\}$ is ergodic for $[x,\theta|y]$.

"Monte Carlo is an extremely bad method; it should be used only when all alternative methods are worse." (Alan Sokal)

Marginal Posterior over Hyperparameters $[\theta|y]$

$$[\theta|y] = \int_X [x,\theta|y]\,\mathrm{d}x$$

Avoid calculating this integral over high-dimensional latent field x.

A cheap algebraic calculation is available when the full conditional for x

$$[x|\theta,y] = \frac{[y|x]\,[x|\theta]}{[y|\theta]}$$

has known form. Then the normalising constant $[y|\theta]$ has known θ dependence, and

$$[\theta|y] \propto [y|\theta]\,[\theta].$$

R. A. Norton, J. A. Christen, and C. Fox. Sampling hyperparameters in hierarchical models: improving on Gibbs for high-dimensional latent fields and large datasets. *Communications in Statistics - Simulation and Computation*, 47(9):2639–2655, 2018.

Markov chain Monte Carlo

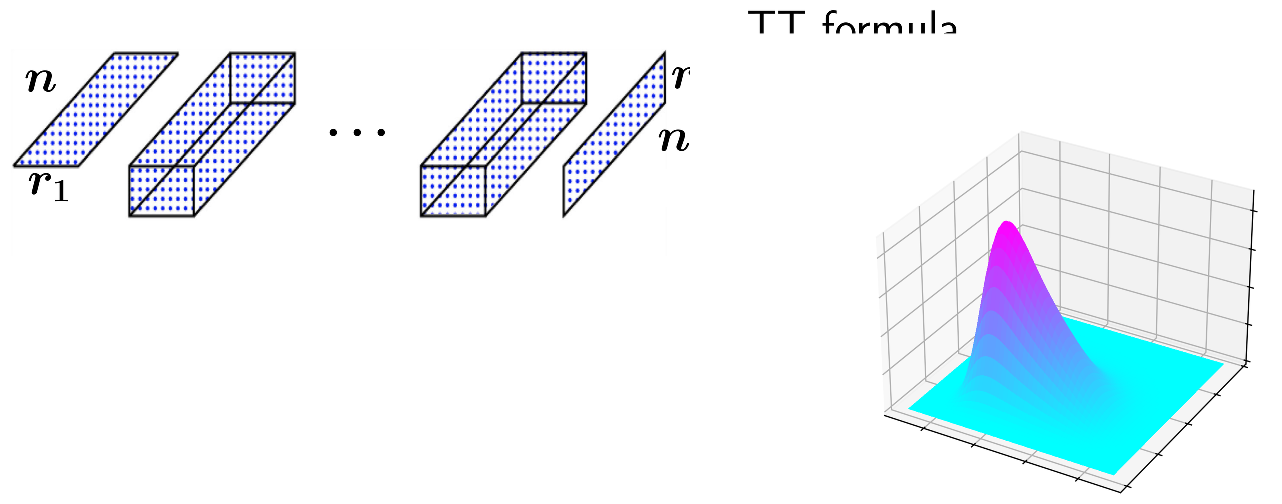
A representative MCMC scheme is the block Gibbs sampler

- Draw $\theta' \sim [\theta|x]$
- Draw $x' \sim [x|\theta',y]$

simulating a transition kernel that targets the posterior $[x,\theta|y]$.
Narrow scatter plot shows why this is slow –

Better is to move in the marginal posterior over hyperparameters $[\theta|y]$
H. Rue and L. Held. *Gaussian Markov random fields : Theory and applications.* Chapman Hall, New York, 2005.

Tensor Train Representation of $[\theta|y]$



$$f_{X_k}(x_k) = \frac{1}{z}\left(\gamma'\prod_{i=1}^{k-1}\lambda_i(X_i)\prod_{i=k+1}^{d}\lambda_i(X_i) + \sum_{l_{k-1}=1}^{r_{k-1}}\sum_{l_k=1}^{r_k}\left(\sum_{i=1}^{n}\phi_k^{(i)}(x_k)D_k[l_{k-1},i,l_k]\right)^2\right)\lambda_k(x_k)$$

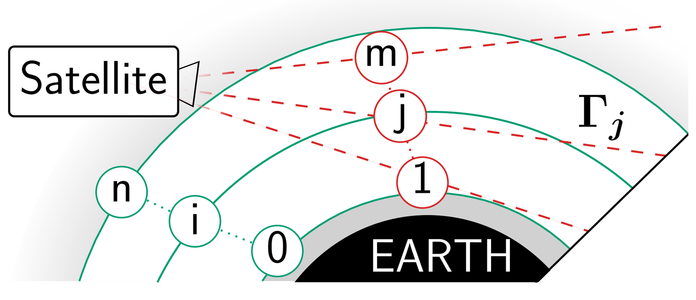
S. Dolgov, K. Anaya-Izquierdo, C. Fox, and R. Scheichl. Approximation and sampling of multivariate probability distributions in the tensor train decomposition. *Statistics and Computing*, 30(3):603–625, 2020.

Independent Posterior Sampling (MTC)

If the inner expectation is not available exactly, draw *independent* posterior samples by: Use TT representation to sample $\theta' \overset{\text{iid}}{\sim} [\theta|y]$ then $x' \sim [x|\theta',y]$

C. Fox and R. A. Norton. Fast sampling in a linear-Gaussian inverse problem. *SIAM/ASA Journal on Uncertainty Quantification*, 4(1):1191–1218, 2016.

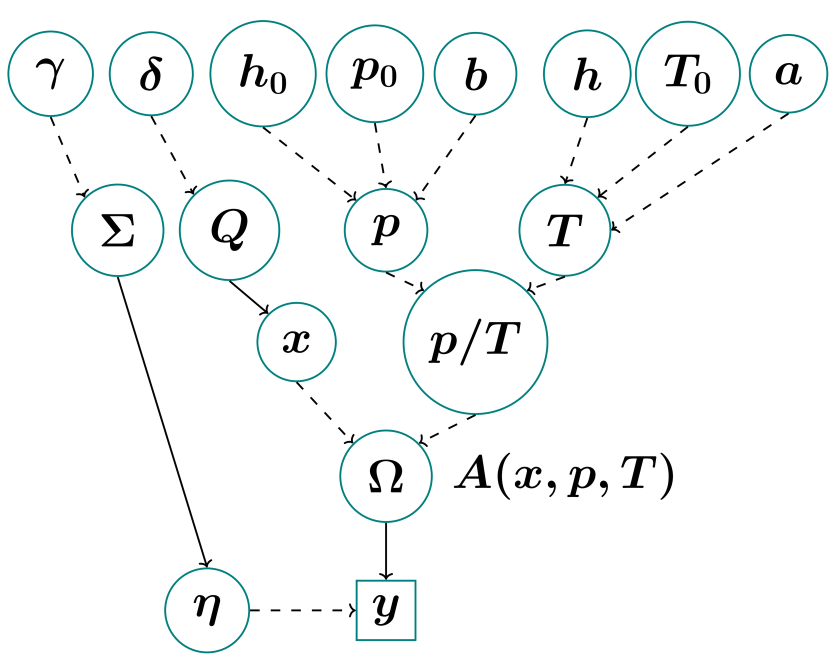
Inverse Problem of Recovering Ozone Profile



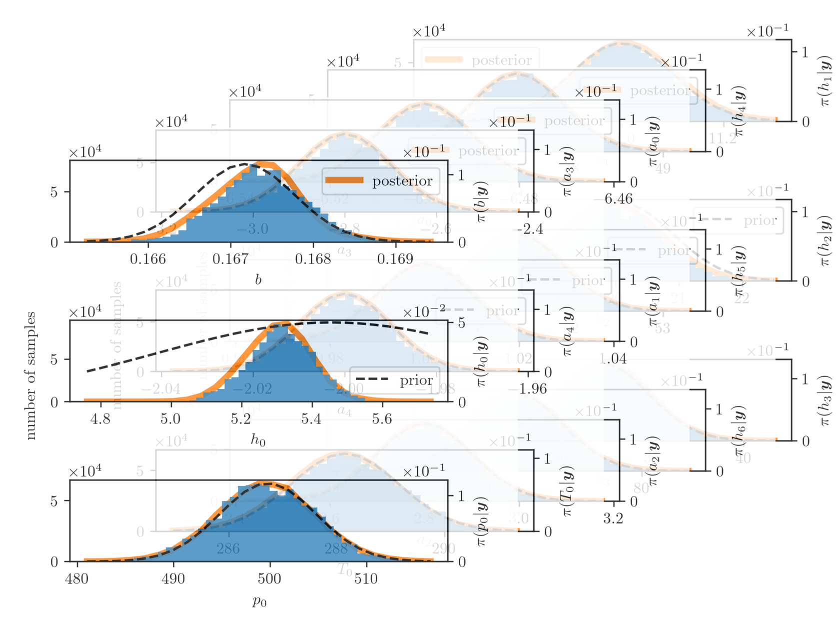
$$y_j = \int_{\Gamma_j} B(\nu,T)k(\nu,T)\frac{p(T)}{k_B T(r)}x(r)\tau(r)\mathrm{d}r + \eta_j$$

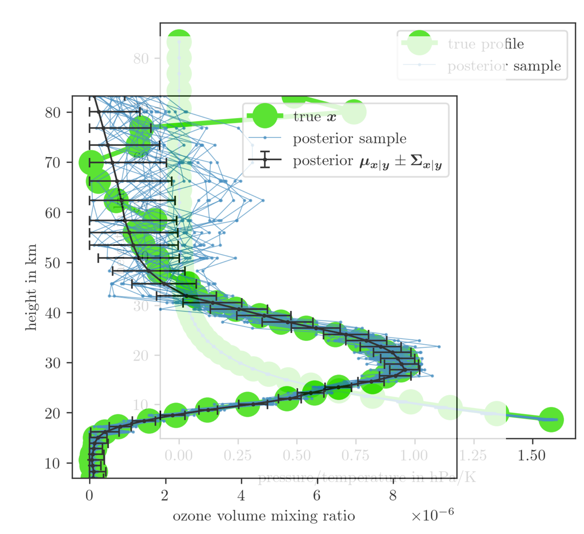
$$\tau(r) = \exp\left\{-\int_{r_{\mathrm{obs}}}^{r} k(\nu,T)\frac{p(T)}{k_B T(r')}x(r')\mathrm{d}r'\right\}$$

$$y = MAx + \eta$$



Posterior Expectation by TT and Affine Representations





- output sumarray
- time
- other stuff