

ML FOR ECONOMETRICIANS

DISTRIBUTED MCMC

Mattias Villani

**Division of Statistics and Machine Learning
Department of Computer and Information Science
Linköping University**



LECTURE OVERVIEW

- ▶ **Parallelism - potential and limitations**
- ▶ **Distributed MCMC**

PARALLELISM - POTENTIAL

- ▶ **Why?** Cores don't get much faster, but we get more of them.
- ▶ **MCMC is serial** - hard to parallelize.
- ▶ **Independence MH** can be parallelized by:
 1. In parallel: generate **all** proposal draws and evaluate posterior densities.
 2. Run Markov Chain on single core using pre-computed quantities from 1.
 3. Inject a random walk step every r :th step to avoid getting stuck.
- ▶ Graphic cards (**GPU**) have thousands of cores.
Hours \rightarrow Seconds in favorable cases. [1, 2, 3]
- ▶ **Conditional independence** can open up parallelism. [4]
- ▶ Special solutions: **Pre-fetching**. Predict the future state of the MCMC chain and pre-compute ahead of time. [5, 6]

PARALLELISM - LIMITATIONS

- ▶ Need special code. **Harder to debug.**
- ▶ Graphic cards (**GPU**) requires very careful data management to be really effective. RAM/Shared/Constant/Registers. See the MCMC in [3]
- ▶ **Avoiding marginalization** \Rightarrow Conditional independences \Rightarrow Parallelism, but can slow down convergence. But not always. Terenin et al (2017).
- ▶ **Amdahl's law.** 'The theoretical speedup is always limited by the part of the task that cannot benefit from the improvement'.
- ▶ **Communication overhead** limits gains from parallelism. Asynchronous MCMC may help. [7]
- ▶ The data set may be **larger than RAM** memory.

DISTRIBUTED MCMC

- ▶ **Map-Reduce** philosophy: bring the computations to the data.
- ▶ General idea:
 - ▶ **Split** the data across many machines.
 - ▶ **Run separate** MCMC chains on each machine. **Subposteriors**.
 - ▶ **Combine** the MCMC **draws** after the MCMC.
- ▶ Posterior and subposteriors from S machines/data subsets

$$p(\theta|\mathbf{y}) \propto \prod_{s=1}^S p(\mathbf{y}_s|\theta)p(\theta)^{1/S}$$

- ▶ The subsets $\mathbf{y}_1, \dots, \mathbf{y}_S$ are assumed **conditionally independent**.
- ▶ $p(\theta) = \prod_{s=1}^S p(\theta)^{1/S}$ to preserve total prior information.
Make sure that $p(\theta)^{1/S}$ is proper!
- ▶ **How to combine draws** from different subposteriors?

CONSENSUS MONTE CARLO

- **Assume** that each subposterior $p(\theta|\mathbf{y}_s)$ is $N(\mu_s, \Omega_s)$. Then

$$p(\theta|\mathbf{y}) \propto \prod_{s=1}^S p(\theta|\mathbf{y}_s) = N(\mu, \Omega)$$

where

$$\Omega^{-1} = \sum_{s=1}^S \Omega_s^{-1} \quad \mu = \Omega \left(\sum_{s=1}^S \Omega_s^{-1} \mu_s \right)$$

- Scott et al. (2013) [8] therefore propose to take (matrix) **weighted averages of the subposterior draws**:

$$\theta^{(i)} = \left(\sum_{s=1}^S \Omega_s^{-1} \right)^{-1} \sum_{s=1}^S \Omega_s^{-1} \theta_s^{(i)}, \quad i = 1, \dots, N$$

- Check: $\mathbb{E}(\theta^{(i)}) = \mu$ and $\mathbb{C}(\theta^{(i)}) = \Omega$.

CONSENSUS MONTE CARLO, CONT.

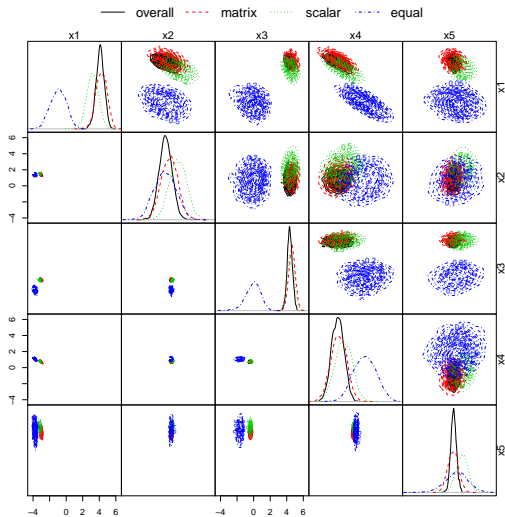
- ▶ The averaging of draws

$$\theta^{(i)} = \left(\sum_{s=1}^S \Omega_s^{-1} \right)^{-1} \sum_{s=1}^S \Omega_s^{-1} \theta_s^{(i)}$$

is **only formally correct when** each subposterior is normal.

- ▶ Posteriors are asymptotically normal (Bernstein-von Mises), but note that it need to hold for each subposterior.
- ▶ Ω_s can be estimated by the sample covariance of $\theta_s^{(1)}, \dots, \theta_s^{(N)}$.
Simplification: assume Ω_s to be diagonal.

LOGISTIC REGRESSION 100 OBS PER MACHINE

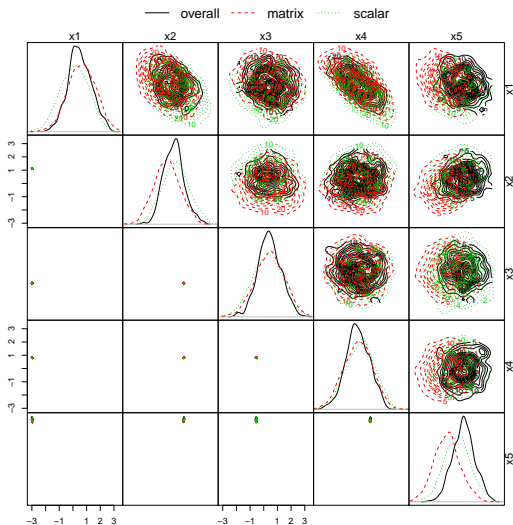


From Scott et al. (2013) [8]

MATTIAS VILLANI (STIMA, LiU)

ML FOR ECONOMETRICS

LOGISTIC REGRESSION 1000 OBS PER MACHINE

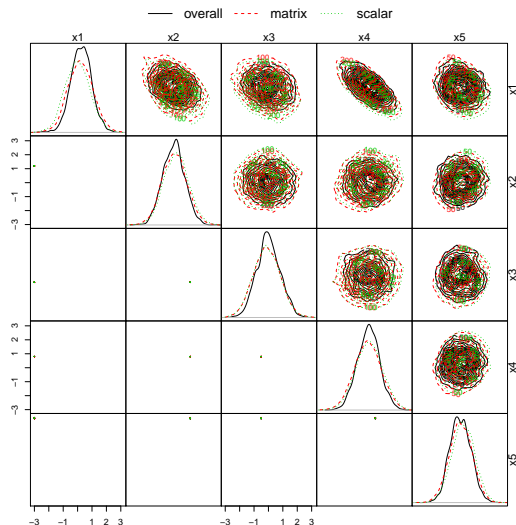


From Scott et al. (2013) [8]

MATTIAS VILLANI (STIMA, LiU)

ML FOR ECONOMETRICS

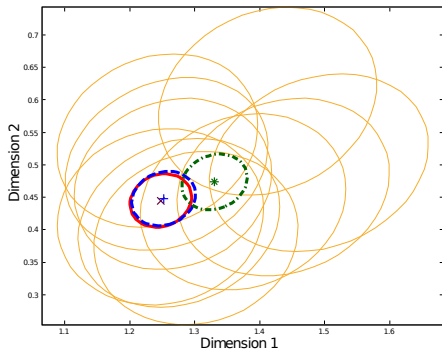
LOGISTIC REGRESSION 10000 OBS PER MACHINE



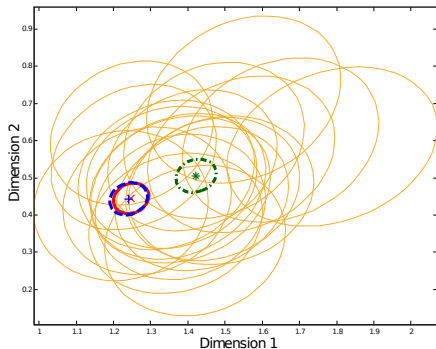
KERNEL-BASED APPROACHES AND COUSINS

- ▶ Neiswanger et al. (2013) [9]
 - ▶ **Nonparametric**. Estimates each subposterior by a kernel density estimator.
 - ▶ **Semiparametric**. Estimates each subposterior by the semiparametric density estimator in Hjort and Glad (1995) [10].
- ▶ **Yin Yang sampler** (Posekany and Fruhwirth-Schnatter, in progress).
- ▶ **Weierstrass sampler** (Wang and Dunson, 2013) [11]
- ▶ Hard to estimate KDEs in moderate to high dimensions.

CONSENSUS MC vs NONPARAMETRIC



- Subposteriors ($M=10$)
- Posterior
- Subposterior Density Product
- Subposterior Average



- Subposteriors ($M=20$)
- Posterior
- Subposterior Density Product
- Subposterior Average

From Neiswanger et al. (2013) [9]

MEDIAN SUBPOSTERIOR (MINSKER ET AL) [12]

► Algorithm:

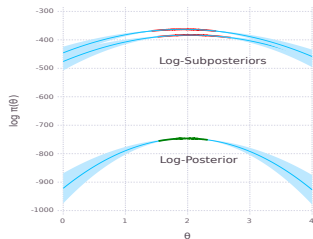
- Run **MCMC on scaled subposteriors** (each of the data observations are replicated S times to mimic the posterior spread).
- Return the **median subposterior** of the S subposteriors.
- Note: the **median is over a space of probability distribution** using some suitable metric. Uniform distribution over atoms $\mathbf{x}_1, \dots, \mathbf{x}_m$:

$$\mathbf{x}_{median} \equiv \operatorname{argmin}_{\mathbf{x} \in \mathcal{X}} \sum_{i=1}^m \|\mathbf{x} - \mathbf{x}_i\|$$

- The median is computed by an efficient algorithm. End result: weights on the subposteriors (draws).
- The median subposterior has two **advantages**:
 - it is a better approximation of the full posterior than the individual subposteriors.
 - it is more **resistant to outliers**.

COMBINING SUBPOSTERIOR USING GPs

- ▶ Main idea in Nemeth and Sherlock (2016) [13]:
 - ▶ use the subposterior MCMC draws **and** the evaluated log-subposterior densities to **fit a GP to each log-subposterior**.
 - ▶ Approximate the full log-posterior by **summing the log-subposterior GPs** (sum of GPs is a GP, just like a sum of Gaussians is Gaussian).
- ▶ **Posterior distribution of the log posterior density function** (a GP is a distribution over functions), including uncertainty.
- ▶ **Prior mean: the subposterior is Gaussian.** Covariance of Gaussian is obtained from MCMC.



COMBINING SUBPOSTERIOR USING GPs

► Algorithm:

- **Run MCMC on each subposterior.** Save draws $\theta_s^{(i)}$ and $\log p(\theta_s^{(i)} | \mathbf{y}_s)$ evaluations, for $i = 1, \dots, I$. Let $\mathcal{D}_s = \left\{ \theta_s^{(1:I)}, \log p(\theta_s^{(1:I)} | \mathbf{y}_s) \right\}$.
- **Fit a noise-free GP regression** to \mathcal{D}_s with response $\log p(\theta_s^{(1:I)} | \mathbf{y}_s)$. Predictive distribution for the log subposterior at a new set of parameter values $\theta^{(1:J)}$

$$\log p_s(\theta^{(1:J)}) | \mathcal{D}_s \sim GP \left(\mu_s(\theta^{(1:J)}), \Sigma_s(\theta^{(1:J)}) \right)$$

- **Sum subposterior GPs** to approximate the full data $\log p(\theta | \mathbf{y})$

$$\log p(\theta^{(1:J)} | \mathbf{y}) | \mathcal{D} \sim GP \left(\sum_{s=1}^S \mu_s(\theta^{(1:J)}), \sum_{s=1}^S \Sigma_s(\theta^{(1:J)}) \right)$$

GP-HMC SAMPLER

- ▶ **Posterior mean** of $p(\theta|\mathbf{y})|\mathcal{D}$ (using properties of log normal)

$$\hat{p}_E(\theta|\mathbf{y}) \equiv \mathbb{E}(p(\theta|\mathbf{y})|\mathcal{D}) = \exp\left(\sum_{s=1}^S \mu_s(\theta) + \frac{1}{2} \sum_{s=1}^S \Sigma_s(\theta)\right)$$

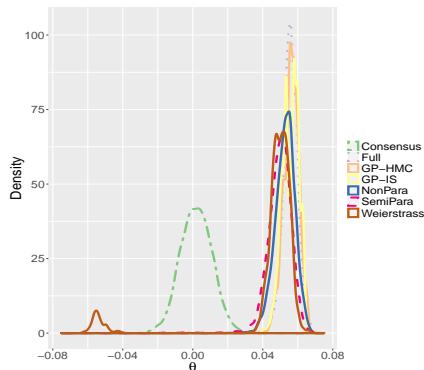
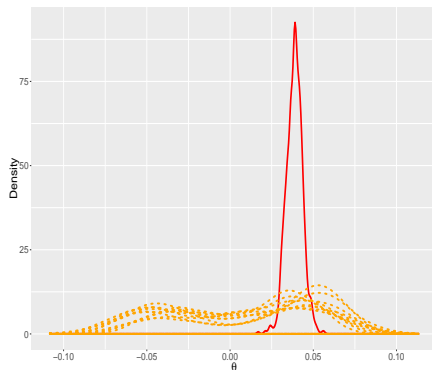
- ▶ **Sample** $\hat{p}_E(\theta|\mathbf{y})$ using **Hamiltonian Monte Carlo (HMC)** on a single machine.
 - ▶ $\hat{p}_E(\theta|\mathbf{y})$ does not depend on the original data. No need to transfer data from the subposterior machines.
 - ▶ $\hat{p}_E(\theta|\mathbf{y})$ relatively cheap to evaluate.
 - ▶ The costly leap-frog steps in HMC are cheap since gradients of $\log \hat{p}_E(\theta|\mathbf{y})$ are available in convenient closed form.

DISTRIBUTED IMPORTANCE SAMPLING

- ▶ Nemeth and Sherlock (2016) [13]: **distributed importance sampler** to **correct any** combination approach.
- ▶ Algorithm:
 - ▶ On central machine: propose $\theta^{(1:N)}$ from joint proposal distribution $q(\theta^{(1:N)})$ with identical marginals $q_1(\theta^{(i)})$.
 - ▶ Transfer $\theta^{(1:N)}$ to all submachines.
 - ▶ Evaluate $p(\theta^{(1:N)} | \mathbf{y}_s)$ on each submachine and return to central machine.
 - ▶ Compute weights on each draw $w_i = \prod_{s=1}^S p(\theta^{(i)} | \mathbf{y}_s) / q_1(\theta^{(i)})$.
 - ▶ Output a weighted posterior sample $\left\{ \theta^{(i)}, w_i \right\}_{i=1}^N$.
- ▶ Unweighted posterior sample by iid sampling from $\left\{ \theta^{(i)}, w_i \right\}_{i=1}^N$.
- ▶ $q(\theta^{(1:N)})$ is iid Gaussian in the consensus approach.
- ▶ $q(\theta^{(1:N)})$ sampled by HMC in the GP-HMC sampler.

MIXTURE OF LAPLACE EXAMPLE [13]

- ▶ Simulated data set from mixture of two Laplace distributions.
- ▶ 1M observations. 1 parameter. $S = 20$ machines.



From Nemeth and Sherlock (2016) [13]

MIXTURE OF LAPLACE EXAMPLE

Algorithm	$D_{Mah.}$	$D_{KL}(\pi \hat{\pi})$
Consensus	13.46 (5.62)	5.73 (5.27)
Nonparametric	1.69 (1.66)	0.26 (0.18)
Semiparametric	2.39 (1.79)	0.77 (0.46)
Weierstrass	6.52 (1.76)	0.99 (0.75)
GP-HMC sampler	1.10 (0.96)	0.15 (0.13)
GP-IS sampler	1.62	0.63

From Nemeth and Sherlock (2016) [13]

LOGISTIC REGRESSION EXAMPLE

- ▶ HEPMASS data set.
- ▶ 1M observations.
- ▶ 27 parameters.
- ▶ $S = 20$ machines.

Algorithm	$D_{Mah.}$	$D_{KL}(\pi \hat{\pi})$
Consensus	6.13 (5.80)	13.65 (13.22)
Nonparametric	10.73 (5.59)	17.23 (15.76)
Semiparametric	5.36 (5.14)	15.93 (15.01)
Weierstrass	6.48 (4.62)	14.75 (13.98)
GP-HMC sampler	5.90 (5.27)	13.28 (13.57)
GP-IS sampler	6.07	13.56

From Nemeth and Sherlock (2016) [13]



A. Lee, C. Yau, M. B. Giles, A. Doucet, and C. C. Holmes, “On the utility of graphics cards to perform massively parallel simulation of advanced monte carlo methods,” *Journal of computational and graphical statistics*, vol. 19, no. 4, pp. 769–789, 2010.



M. A. Suchard, Q. Wang, C. Chan, J. Frelinger, A. Cron, and M. West, “Understanding gpu programming for statistical computation: Studies in massively parallel massive mixtures,” *Journal of Computational and Graphical Statistics*, vol. 19, no. 2, pp. 419–438, 2010.



A. Eklund, P. Dufort, M. Villani, and S. LaConte, “Broccoli: Software for fast fmri analysis on many-core cpus and gpus,” *Recent Advances and the Future Generation of Neuroinformatics Infrastructure*, p. 208, 2015.



M. Magnusson, L. Jonsson, M. Villani, and D. Broman, “Parallelizing lda using partially collapsed gibbs sampling,” *arXiv preprint arXiv:1506.03784*, 2015.



I. Strid, “Efficient parallelisation of metropolis–hastings algorithms using a prefetching approach,” *Computational Statistics & Data Analysis*, vol. 54, no. 11, pp. 2814–2835, 2010.



M. Banterle, C. Grazian, and C. P. Robert, “Accelerating metropolis-hastings algorithms: Delayed acceptance with prefetching,” *arXiv preprint arXiv:1406.2660*, 2014.



A. Terenin, D. Simpson, and D. Draper, “Asynchronous distributed gibbs sampling,” *arXiv preprint arXiv:1509.08999*, 2015.



S. L. Scott, A. W. Blocker, F. V. Bonassi, H. Chipman, E. George, and R. McCulloch, “Bayes and big data: the consensus Monte Carlo algorithm,” in *Bayes 250 conference*, vol. 16, 2013.



W. Neiswanger, C. Wang, and E. Xing, “Asymptotically exact, embarrassingly parallel MCMC,” *arXiv preprint arXiv:1311.4780*, 2013.



N. L. Hjort and I. K. Glad, “Nonparametric density estimation with a parametric start,” *The Annals of Statistics*, pp. 882–904, 1995.



X. Wang and D. B. Dunson, “Parallel MCMC via Weierstrass sampler,” *arXiv preprint arXiv:1312.4605*, 2013.



S. Minsker, S. Srivastava, L. Lin, and D. Dunson, “Scalable and robust Bayesian inference via the median posterior,” in *Proceedings of the 31st International Conference on Machine Learning (ICML-14)*, pp. 1656–1664, 2014.



C. Nemeth and C. Sherlock, “Merging mcmc subposteriors through gaussian-process approximations,” *arXiv preprint arXiv:1605.08576*, 2016.