Markov Chain Monte Carlo algorithms

Modèles probabilistes pour l'apprentissage

Théo Moins[1]

[1]Statify, Inria Grenoble Rhône-Alpes

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Reminder: Bayesian paradigm

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What's next?

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What's next? All computations reduce to posterior means of quantity of interest $f(\boldsymbol{\theta})$:

$$\mathbb{E}_{p(\cdot \mid \mathbf{x})}[f(\boldsymbol{\theta})] = \int f(\boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathbf{x}) d\boldsymbol{\theta}$$

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(highly dimensional, non-explicit, etc.)

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Monte Carlo	Markov Chain
$\mathbb{E}[f(\boldsymbol{\theta})] \approx \frac{1}{N}\sum_{i=1}^{N} f(\boldsymbol{\theta}^{(i)})$	$\boldsymbol{\theta}^{(i+1)} \mid \boldsymbol{\theta}^{(i)} \sim P(\boldsymbol{\theta}^{(i)}, \cdot)$

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With a correct choice of $P(\cdot, \cdot)$ one can often prove that

$$\frac{1}{N}\sum_{i=1}^{N} f(\boldsymbol{\theta}^{(i)}) \to \mathbb{E}_{p(\cdot|\mathbf{x})}[f(\boldsymbol{\theta})], \quad \text{when } N \to +\infty.$$

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Metropolis–Hastings

Initialize $\boldsymbol{\theta}^{(0)}$;
for $i \leftarrow 1$ **to** N **do**
  Sample a candidate $\boldsymbol{\theta}^* \sim q(\boldsymbol{\theta}^* | \boldsymbol{\theta}^{(i-1)})$;
  Compute an acceptation ratio $\alpha(\boldsymbol{\theta}^* \mid \boldsymbol{\theta}^{(i-1)}) \in [0, 1]$;
  Accept the candidate $(\boldsymbol{\theta}^{(i)} = \boldsymbol{\theta}^*)$ with probability $\alpha(\boldsymbol{\theta}^* \mid \boldsymbol{\theta}^{(i-1)})$;
  Otherwise reject $(\boldsymbol{\theta}^{(i)} = \boldsymbol{\theta}^{(i-1)})$;
end

Algorithm 1: Metropolis-Hastings Algorithm

Illustration: `https://chi-feng.github.io/mcmc-demo/app.html`

Metropolis–Hastings

Acceptation ratio for the general framework:

$$\alpha(\boldsymbol{\theta}^* \mid \boldsymbol{\theta}^{(i-1)}) = \min\left(1, \frac{p(\boldsymbol{\theta}^*|\mathbf{x})}{p(\boldsymbol{\theta}^{(i)}|\mathbf{x})} \frac{q(\boldsymbol{\theta}^{(i)}|\boldsymbol{\theta}^*)}{q(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(i)})}\right)$$

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Special cases:

- **Metropolis**: $q(\boldsymbol{\theta}^{(i)}|\boldsymbol{\theta}^*) = q(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(i)})$ (symmetrical proposal).

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Special cases:

- **Metropolis**: $q(\boldsymbol{\theta}^{(i)}|\boldsymbol{\theta}^*) = q(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(i)})$ (symmetrical proposal).
- **Gibbs**: $q(\theta_k^*|\boldsymbol{\theta}^{(i)}) = p(\theta_k^*|\theta_1^{(i)}, \cdots, \theta_D^{(i)}, \mathbf{x})$ (full conditional, $\alpha(\boldsymbol{\theta}^* \mid \boldsymbol{\theta}^{(i-1)}) = 1$)

Metropolis–Hastings

```
Initialize θ^(0);
for i ← 1 to N do
    Sample θ* ~ q(θ*|θ^(i−1));
    Sample u ~ U[0, 1];
    if u < α(θ* | θ^(i−1)) then
        θ^(i) = θ*                                  /* Accept */
    else
        θ^(i) = θ^(i−1)                             /* Reject */
    end
end
```

Algorithm 2: Metropolis–Hastings Algorithm

Performance of Random Walk Metropolis

To conclude:

1. **Proposal distribution** $q(\boldsymbol{\theta}^*|\boldsymbol{\theta}^{(i-1)})$: favour large volumes ...

2. **Acceptance ratio** $\alpha(\boldsymbol{\theta}^* \mid \boldsymbol{\theta}^{(i-1)})$: favour large densities.

$\implies$ The combination makes the selection toward the typical set.

Drawback: tuning is extremely hard in high dimension!

MCMC

To sum up:

MCMC algorithms

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- Iterative sampling of the probability density,
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- Based on an Acceptation-Rejection Rule,
- Examples: Metropolis-Hastings (MH), Gibbs Sampler, Hamiltonian Monte Carlo (HMC) etc.

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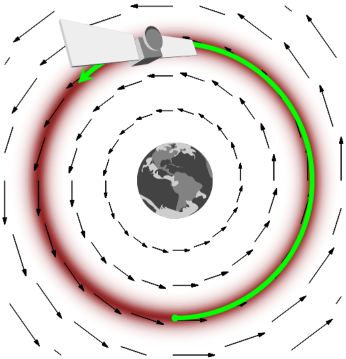
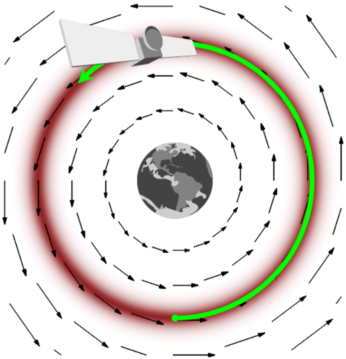
Introduction to HMC



From Betancourt (2017)

Introduction to HMC

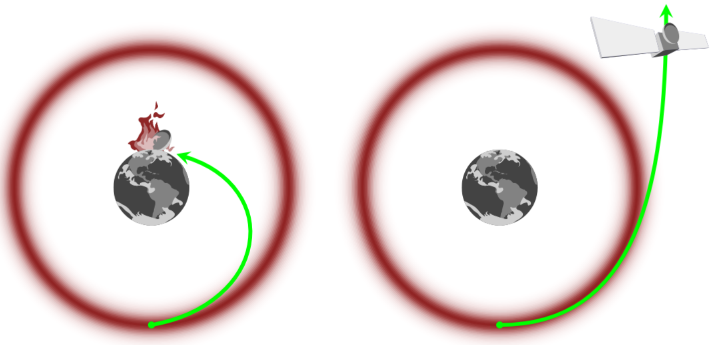


From Betancourt (2017)

- Probabilistic system $\rightarrow$ Physical system
- Mode of the distribution $\rightarrow$ Massive planet
- Gradient of the density $\rightarrow$ Gravitational field

Introduction to HMC

Conservative exploration:



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$$\implies p(\boldsymbol{\theta}, \boldsymbol{\xi} \mid \mathbf{x}) = p(\boldsymbol{\xi} \mid \boldsymbol{\theta}, \mathbf{x}) p(\boldsymbol{\theta} \mid \mathbf{x})$$

Hamiltonian definition:

$$\begin{aligned} H(\boldsymbol{\theta}, \boldsymbol{\xi}) &= -\log p(\boldsymbol{\xi}, \boldsymbol{\theta} \mid \mathbf{x}) \\ &= -\log p(\boldsymbol{\xi} \mid \boldsymbol{\theta}, \mathbf{x}) - \log p(\boldsymbol{\theta} \mid \mathbf{x}) \\ &= \qquad K \qquad + \qquad V, \qquad \text{with} \begin{cases} K : & \text{kinetic energy} \\ V : & \text{potential energy} \end{cases} \end{aligned}$$

Introduction to HMC

Hamilton's equation of motion:

$$\frac{d\theta_k}{dt} = \frac{\partial H}{\partial \xi_k}, \qquad \frac{d\xi_k}{dt} = \frac{\partial H}{\partial \theta_k}. \tag{1}$$

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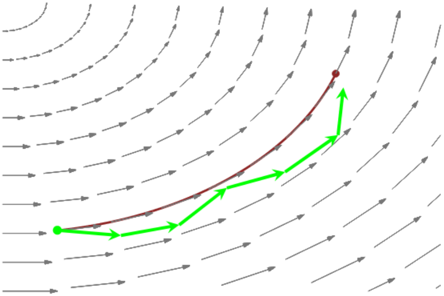
Solving (1) leads to obtain the position $\phi_t(\boldsymbol{\theta}, \boldsymbol{\xi}) \in \mathbb{R}^{2D}$ accross time t.



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Initialize $\boldsymbol{\theta}^{(0)}$;
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    Sample a momentum $\boldsymbol{\xi}^{(i-1)} \sim q(\boldsymbol{\xi}^{(i-1)} \mid \boldsymbol{\theta}^{(i-1)})$;
    Sample an amount of time $t \sim \mathcal{U}[0, T]$;
    Numerically solve the Hamilton's equation $(\boldsymbol{\theta}_t, \boldsymbol{\xi}_t) \leftarrow \phi_t(\boldsymbol{\theta}^{(i-1)}, \boldsymbol{\xi}^{(i-1)})$;
    Accept the candidate $(\boldsymbol{\theta}^{(i)} = \boldsymbol{\theta}_t)$ with probability $\alpha(\boldsymbol{\theta}_t, -\boldsymbol{\xi}_t \mid \boldsymbol{\theta}^{(i-1)}, \boldsymbol{\xi}^{(i-1)})$;
    Otherwise reject $(\boldsymbol{\theta}^{(i)} = \boldsymbol{\theta}^{(i-1)})$;
end

Algorithm 3: HMC Algorithm

Introduction to HMC

Initialize $\boldsymbol{\theta}^{(0)}$;

for $i \leftarrow 1$ **to** N **do**

  Sample $\boldsymbol{\xi}^* \sim \mathcal{N}(0, M)$;

  Let $\boldsymbol{\theta}_0 = \boldsymbol{\theta}^{(i-1)}$ and $\boldsymbol{\xi}_0 = \boldsymbol{\xi}^*$;

  for $l \leftarrow 1$ **to** L **do**

    $\boldsymbol{\xi}_{l-1/2} = \boldsymbol{\xi}_{l-1} - \epsilon \nabla_{\boldsymbol{\theta}} V(\boldsymbol{\theta}_0)/2$;

    $\boldsymbol{\theta}_l = \boldsymbol{\theta}_{l-1} + \epsilon \boldsymbol{\xi}_{l-1}$;

    $\boldsymbol{\xi}_l = \boldsymbol{\xi}_{l-1/2} - \epsilon \nabla_{\boldsymbol{\theta}} V(\boldsymbol{\theta}_{Leaps})/2$;

  end

  Sample $u \sim \mathcal{U}[0, 1]$;

  if $u < \alpha(\boldsymbol{\theta}_L, -\boldsymbol{\xi}_L \mid \boldsymbol{\theta}_0, \boldsymbol{\xi}_0)$ **then**

    $\boldsymbol{\theta}^{(i)} = \boldsymbol{\theta}_L$ `/* Accept */`

  else

    $\boldsymbol{\theta}^{(i)} = \boldsymbol{\theta}_0$ `/* Reject */`

  end

Introduction to HMC - Summary

Hamiltonian Monte Carlo

- Algorithm based on Hamiltonian Mechanics
- Time discretization simulated by the Leap Frog Algorithm
- Acceptation rule based on the discretization error in simulating Hamiltonian mechanics
- A lot of hyperparameters!

References:

Betancourt, M. (2017). A conceptual introduction to Hamiltonian Monte Carlo. *arXiv preprint arXiv:1701.02434*.

Gelman, A. and Rubin, D. B. (1992). Inference from iterative simulation using multiple sequences. *Statistical science*, 7(4):457–472.

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Bayesian inference on $\boldsymbol{\theta} \sim p(\boldsymbol{\theta} \mid \mathbf{x}) \implies$ computation of $\mathbb{E}_{p(\cdot \mid \mathbf{x})}[f(\boldsymbol{\theta})] = \int f(\boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \mathbf{x}) d\boldsymbol{\theta}$.

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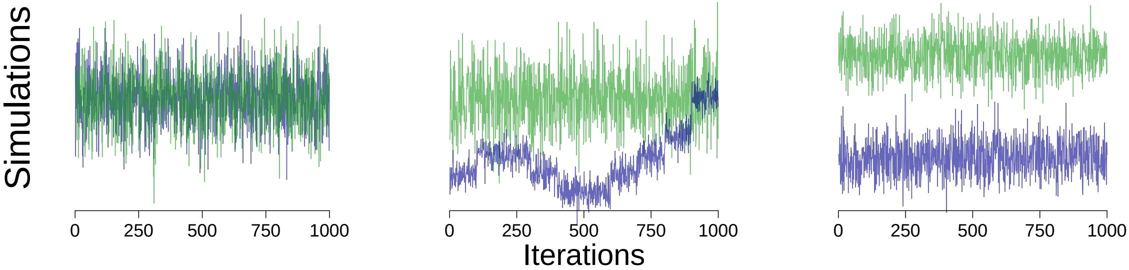
With a correct choice of $P(\cdot, \cdot)$ one can often prove that

$$\frac{1}{N} \sum_{i=1}^{N} f(\boldsymbol{\theta}^{(i)}) \to \mathbb{E}_{p(\cdot|\mathbf{x})}[f(\boldsymbol{\theta})], \quad \text{when } N \to +\infty.$$

$\hookrightarrow$ How to choose N?

Has the chain(s) converged?

Two kind of convergence issues: mixing and stationarity (univariate case)



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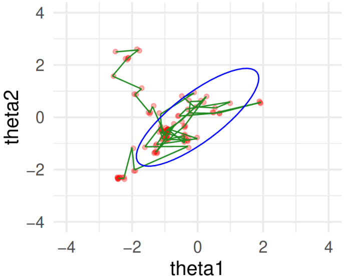

From Aki Vehtari : https://avehtari.github.io/BDA_course_Aalto/

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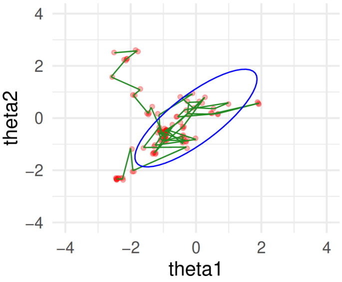

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Warm-up: discard the early iterations (usually the first half),

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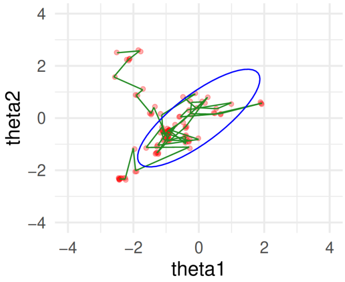

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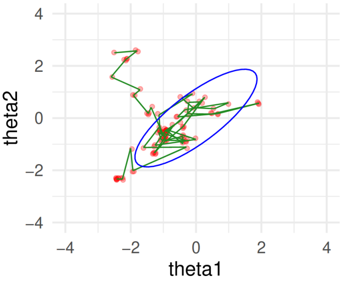

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Warm-up: discard the early iterations (usually the first half),
Thinning: keep every kth iterations from each sequence,
Multiple chains: reduce the influence of the starting point.

Autocorrelation

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Autocorrelation function at lag-t: correlation between elements of the sequence distant from t steps.

$$\mathrm{ACF}_t(\theta) = \frac{\mathrm{ACov}_t(\theta)}{\mathrm{Var}(\theta)} = \frac{\frac{1}{S-t}\sum_{s=1}^{S-t}(\theta^{(s)} - \overline{\theta})(\theta^{(s+t)} - \overline{\theta})}{\frac{1}{S-1}\sum_{s=1}^{S}(\theta^{(s)} - \overline{\theta})^2}$$

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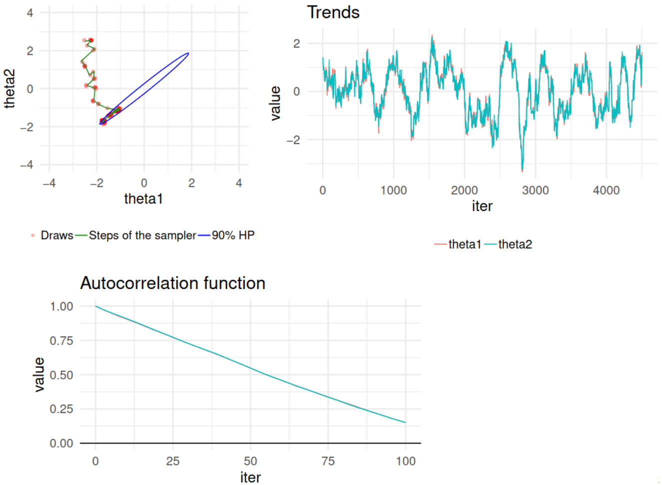
Ideal case: uncorrelated draws $\implies \mathrm{ACF}_t(\theta) = 0 \quad \forall t > 1$

Autocorrelation



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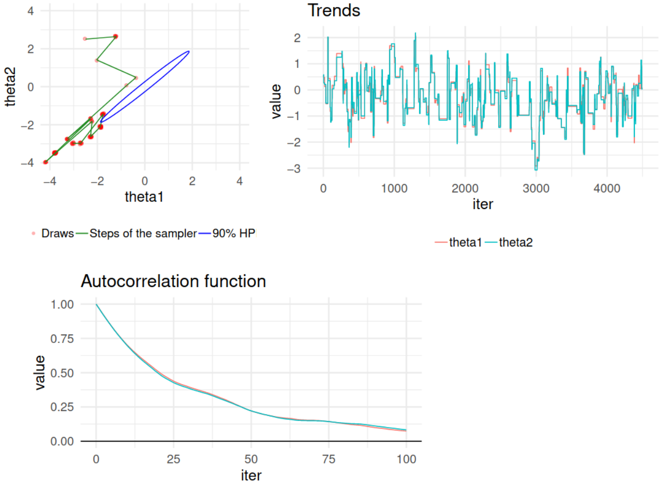

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Effective Sample Size (ESS)

In the independent case ($M = 1$ chain):

$$N.\mathrm{Var}(\overline{\theta}) = N.\mathbb{E}\left[(\overline{\theta} - \theta_0)^2\right] \xrightarrow[n \to +\infty]{} \mathrm{Var}(\theta \mid \boldsymbol{x})$$

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Otherwise:

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ESS: Equivalent number of independent draws

$$\mathrm{ESS} = \frac{N}{1 + 2\sum_{t=1}^{N} \mathrm{ACF}_t(\theta)}$$

$\hookrightarrow$ Number of samples to obtain the same variance in the i.i.d case.

$\hat{R}$ (aka potential scale reduction factor)

Introduced by Gelman and Rubin (1992).
Consider m chains of size n, with $\theta^{(i,j)}$ denoting the ith draw from chain j.
Comparison of the **between-variance** B and the **within-variance** W of the chains:

$$\hat{R} = \sqrt{\frac{\hat{W} + \hat{B}}{\hat{W}}}$$

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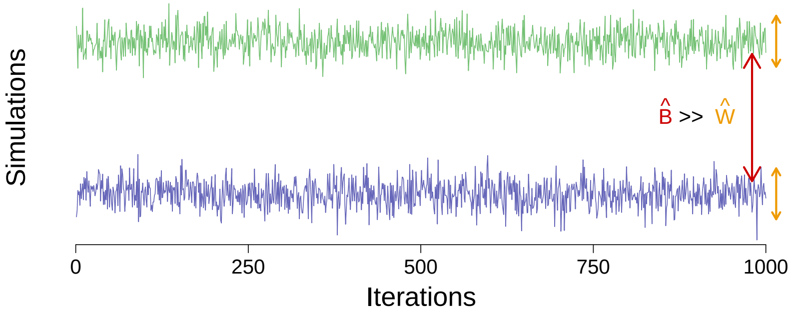
$$\text{Between var}: \hat{B} = \frac{1}{m-1}\sum_{j=1}^{m}(\bar{\theta}^{(\cdot,j)} - \bar{\theta}^{(\cdot,\cdot)})^2, \quad \text{where } \bar{\theta}^{(\cdot,j)} = \frac{1}{n}\sum_{i=1}^{n}\theta^{(i,j)}, \quad \bar{\theta}^{(\cdot,\cdot)} = \frac{1}{m}\sum_{j=1}^{m}\bar{\theta}^{(\cdot,j)},$$

$$\text{Within var}: \hat{W} = \frac{1}{m}\sum_{j=1}^{m}s_j^2, \quad \text{where } s_j^2 = \frac{1}{n-1}\sum_{i=1}^{n}(\theta^{(i,j)} - \bar{\theta}^{(\cdot,j)})^2.$$

$\hat{R}$ (aka potential scale reduction factor)

Introduced by Gelman and Rubin (1992).
Consider m chains of size n, with $\theta^{(i,j)}$ denoting the ith draw from chain j.
Comparison of the **between-variance** B and the **within-variance** W of the chains:

$$\hat{R} = \sqrt{\frac{\hat{W} + \hat{B}}{\hat{W}}}$$



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BDA book recommends to use $\hat{R}$ and ESS in the following way:

$$\hat{R} \in [1, 1.01] \implies \text{“Chains are mixing well”}.$$
$$ESS > 400 \implies \text{“Enough data for estimation”}.$$

Example 1: Bayesian logistic regression

$$\boldsymbol{\beta} \sim \mathcal{N}(0, 0.35^2.\boldsymbol{I}_4), \quad y_j \sim \text{Bernoulli}\left(\frac{1}{1 + e^{-\boldsymbol{x}_j^\top \boldsymbol{\beta}}}\right).$$

Examples

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Example 2: Hierarchical model (8 Schools)

$\hookrightarrow$ Test the effectiveness of coaching courses.

y_j: coaching effect for the school j

$$\mu \sim \mathcal{N}(0,5), \quad \tau \sim \mathcal{N}(0,10),$$
$$\theta_j \sim \mathcal{N}(\mu,\tau), \quad y_j \sim \mathcal{N}(\theta_j, \sigma_j^2)$$

Model "in between" the separate model and the joint model.

School	Estimated treatment effect, y_j	Standard error of effect estimate, σ_j
A	28	15
B	8	10
C	-3	16
D	7	11
E	-1	9
F	1	11
G	18	10
H	12	18

From BDA book