Predictive information criteria in hierarchical Bayesian models for clustered data

Sophia Rabe-Hesketh & Daniel Furr

Education & Biostatistics
University of California, Berkeley
sophiarh@berkeley.edu

Joint work with Ed Merkle

Psychological Sciences, University of Missouri

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Outline of Talk

- **Predictive information criteria**
  DIC and WAIC with connections to leave-one-out (LOO) cross-validation

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- **Application to IRT**

Targets of predictive information criteria (non-hierarchical Bayesian model)

- Model likelihood: $f(\boldsymbol{y}|\boldsymbol{\theta}) = \prod_{i=1}^{N} f(y_i|\boldsymbol{\theta})$ Model prior: $p(\boldsymbol{\theta})$

[Gelman, Hwang & Vehtari, 2014]

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  - **WAIC**: integrate over $p(\boldsymbol{\theta}|\boldsymbol{y})$, but use **pointwise** predictive densities

$$-2\,\text{log pointwise predictive density} = -2\sum_{i=1}^{N} \log \mathsf{E}_{\boldsymbol{\theta}|\boldsymbol{y}} f(y_i^{\mathsf{r}}|\boldsymbol{\theta})$$

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- Targets are **expectations** of the above over out-of-sample data $\boldsymbol{y}^{\mathsf{r}}$

[Gelman, Hwang & Vehtari, 2014]

DIC (non-hierarchical Bayesian model)

- Expectation of plug-in deviance (pid) over distribution of $\boldsymbol{y}^{\mathsf{r}}$:

$$\text{expected pid} = -2\mathsf{E}_{\boldsymbol{y}^{\mathsf{r}}} \log f(\boldsymbol{y}^{\mathsf{r}}|\widetilde{\boldsymbol{\theta}})$$

[Spiegelhalter, Best, Carlin & van der Linde, 2002]

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- Use within-sample pid and penalize for using data twice

$$\mathsf{DIC} \;=\; -2\log f(\boldsymbol{y}|\widetilde{\boldsymbol{\theta}}) + 2p_{\mathsf{D}}$$

where p_{D} in penalty term is effective number of parameters

$$p_{\mathsf{D}} \;=\; \mathsf{E}_{\boldsymbol{\theta}|\boldsymbol{y}}[-2\log f(\boldsymbol{y}|\boldsymbol{\theta})] - [-2\log f(\boldsymbol{y}|\tilde{\boldsymbol{\theta}})]$$

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- Posterior means estimated as averages over MCMC draws

[Spiegelhalter, Best, Carlin & van der Linde, 2002]

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- -2 expected log pointwise predictive density (elppd) over distribution of $\boldsymbol{y}^{\mathsf{r}}$:

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- Posterior means and variances estimated from MCMC draws
- Asymptotically equivalent to LOO cross-validation (LOO-CV)

LOO-CV and PSIS-LOO (non-hierarchical Bayesian model)

- Same target as WAIC

$$-2\,\mathsf{elppd} = -2\sum_{i=1}^{N} \mathsf{E}_{\boldsymbol{y}^{\mathsf{r}}} \log \mathsf{E}_{\boldsymbol{\theta}|\boldsymbol{y}} f(y_i^{\mathsf{r}}|\boldsymbol{\theta})$$

[Vehtari, Gelman & Gabry, 2017]

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- Estimate using LOO-CV

$$-2\,\mathsf{LOO\text{-}CV} \;=\; -2\sum_{i=1}^{N} \log \mathsf{E}_{\boldsymbol{\theta}|\boldsymbol{y}_{-i}} f(y_i|\boldsymbol{\theta})$$

  - Where $\boldsymbol{y}_{-i}$ is the "training" data without unit i
  - Requires running MCMC on each of N training datasets

[Vehtari, Gelman & Gabry, 2017]

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- Approximate by Pareto-smoothed importance sampling (PSIS)
  - Idea of importance sampling (IS)

$$-2\,\text{IS-LOO} \;=\; -2\sum_{i=1}^{N} \log \mathsf{E}_{\boldsymbol{\theta}|\boldsymbol{y}} \underbrace{\left[\frac{p(\boldsymbol{\theta}|\boldsymbol{y}_{-i})}{p(\boldsymbol{\theta}|\boldsymbol{y})}\right]}_{\text{importance ratio}} f(y_i|\boldsymbol{\theta})$$

  - Importance ratios $\propto \frac{1}{f(y_i|\boldsymbol{\theta})}$; Unstable, hence Pareto smoothing

[Vehtari, Gelman & Gabry, 2017]

Hierarchical Bayesian models for clustered data

Stage	MLM Example
3	
2	
1	

Hierarchical Bayesian models for clustered data

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1	Hyperparameters	hyperprior for ψ

Hierarchical Bayesian models for clustered data

Stage		MLM Example	Densities, general notation	
3	Responses	$y_{ij} \sim N(\alpha + \zeta_j, \sigma^2)$	$f_c(y_{ij}\|\boldsymbol{\omega}, \boldsymbol{\zeta}_j)$	$\boldsymbol{\omega} \equiv (\alpha, \sigma^2)'$
		unit $i = 1, \ldots, n_j$		$\boldsymbol{\zeta}_j \equiv \zeta_j$
2	Direct param.	$\zeta_j \sim N(0, \psi)$	$g(\boldsymbol{\zeta}_j\|\boldsymbol{\psi})$	$\boldsymbol{\psi} \equiv \psi$
		cluster $j = 1, \ldots, J$		
	Fully Bayesian $\downarrow$			
		prior for α, σ^2	$p(\boldsymbol{\omega})$	
1	Hyperparameters	hyperprior for ψ	$p(\boldsymbol{\psi})$	

Hierarchical Bayesian models for clustered data

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- ζ_j are direct parameters, varying intercepts/coefficients (MLM), latent variables (SEM/IRT), missing data

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	Fully Bayesian	$\downarrow$		
		prior for α, σ^2	$p(\boldsymbol{\omega})$	
1	Hyperparameters	hyperprior for ψ	$p(\boldsymbol{\psi})$	

- $\boldsymbol{\zeta}_j$ are direct parameters, varying intercepts/coefficients (MLM), latent variables (SEM/IRT), missing data
- In Bayesian setting, ambiguous whether $\boldsymbol{\zeta}_j$ are parameters or (latent) variables

Revisit DIC
Two versions of the likelihood (or deviance)

- **Conditional likelihood**: $\prod_j f_c(\boldsymbol{y}_j|\boldsymbol{\omega}, \boldsymbol{\zeta}_j)$, where

$$f_c(\boldsymbol{y}_j|\boldsymbol{\omega}, \boldsymbol{\zeta}_j) = \prod_{i=1}^{n_j} f_c(y_{ij}|\boldsymbol{\omega}, \boldsymbol{\zeta}_j)$$

  - Natural definition in `Stan` (or `BUGS`/`JAGS`) code
  - Condition on $\boldsymbol{\omega}$ and $\boldsymbol{\zeta} = (\boldsymbol{\zeta}_1{}', \ldots, \boldsymbol{\zeta}_J{}')'$

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  - Condition on $\boldsymbol{\omega}$ and $\boldsymbol{\zeta} = (\boldsymbol{\zeta}_1{}', \ldots, \boldsymbol{\zeta}_J{}')'$

- **Marginal likelihood**: $\prod_j f_m(\boldsymbol{y}_j|\boldsymbol{\omega}, \boldsymbol{\psi})$, where

$$f_m(\boldsymbol{y}_j|\boldsymbol{\omega}, \boldsymbol{\psi}) = \int f_c(\boldsymbol{y}_j|\boldsymbol{\omega}, \boldsymbol{\zeta}_j) g(\boldsymbol{\zeta}_j|\boldsymbol{\psi}) d\boldsymbol{\zeta}_j$$

  - Natural in maximum likelihood (ML) estimation (e.g., `lmer` in R)
  - Condition on $\boldsymbol{\omega}$ and $\boldsymbol{\psi}$, the only parameters in ML setting
  - In MLM example, $f_m(\boldsymbol{y}_j|\boldsymbol{\omega}, \boldsymbol{\psi})$ is MVN with means α, variances $\psi + \sigma^2$, and covariances ψ

Conditional and marginal DIC

- **Conditional DIC**
  ζ (and ω) "in focus" [Spiegelhalter, Best, Carlin & van der Linde, 2002]

$$\mathsf{DIC_c} \;=\; -2\log f_{\mathsf{c}}(\boldsymbol{y}|\tilde{\boldsymbol{\omega}},\tilde{\boldsymbol{\zeta}}) + 2p_{\mathsf{Dc}}$$

$$p_{\mathsf{Dc}} \;=\; \mathsf{E}_{\boldsymbol{\omega},\boldsymbol{\zeta}|\boldsymbol{y}}[-2\log f_{\mathsf{c}}(\boldsymbol{y}|\boldsymbol{\omega},\boldsymbol{\zeta})] + 2\log f_{\mathsf{c}}(\boldsymbol{y}|\tilde{\boldsymbol{\omega}},\tilde{\boldsymbol{\zeta}})$$

  - Used in almost all application, easy with `Stan`, `BUGS`, `JAGS`

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  - Used in almost all application, easy with `Stan`, `BUGS`, `JAGS`

- **Marginal DIC**
  ψ (and ω) "in focus"

$$\mathsf{DIC_m} \;=\; -2\log f_{\mathsf{m}}(\boldsymbol{y}|\tilde{\boldsymbol{\omega}},\tilde{\boldsymbol{\psi}}) + 2p_{\mathsf{Dm}}$$

$$p_{\mathsf{Dm}} \;=\; \mathsf{E}_{\boldsymbol{\omega},\boldsymbol{\psi}|\boldsymbol{y}}[-2\log f_{\mathsf{m}}(\boldsymbol{y}|\boldsymbol{\omega},\boldsymbol{\psi})] + 2\log f_{\mathsf{m}}(\boldsymbol{y}|\tilde{\boldsymbol{\omega}},\tilde{\boldsymbol{\psi}})$$

  - Provided by R package `blavaan` [Merkle & Rosseel, 2018] for SEM (which evaluates $f_{\mathsf{m}}(\boldsymbol{y}|\boldsymbol{\omega},\boldsymbol{\psi})$ using `lavaan`) and by `Mplus`
  - Efficient adaptive quadrature to evaluate intractable integrals [Furr, 2017; Rabe-Hesketh, Skrondal & Pickles, 2005]

Revisit WAIC
Two versions of predictive distributions

- **Posterior predictive distribution** for new unit in *existing* cluster

$$\mathsf{E}_{\boldsymbol{\omega},\boldsymbol{\zeta}_j|\boldsymbol{y}} f_{\mathsf{c}}(y^{\mathsf{r}}_{ij}|\boldsymbol{\omega},\boldsymbol{\zeta}_j) = \int f_{\mathsf{c}}(y^{\mathsf{r}}_{ij}|\boldsymbol{\omega},\boldsymbol{\zeta}_j) \underbrace{\left[\int p(\boldsymbol{\zeta}_j|\boldsymbol{y}_j,\boldsymbol{\omega},\boldsymbol{\psi})p(\boldsymbol{\omega},\boldsymbol{\psi}|\boldsymbol{y})d\boldsymbol{\psi}\right]}_{p(\boldsymbol{\omega},\boldsymbol{\zeta}_j|\boldsymbol{y})} d\boldsymbol{\omega}d\boldsymbol{\zeta}_j$$

Uses **posterior** for ζ_j $\Rightarrow$ directly influenced by $\boldsymbol{y}_j$
$\Rightarrow$ treats ζ_j and therefore cluster as within-sample

[Gelman, Meng & Stern, 1996]

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  Uses **posterior** for $\boldsymbol{\zeta}_j \Rightarrow$ directly influenced by $\boldsymbol{y}_j$
  $\Rightarrow$ treats $\boldsymbol{\zeta}_j$ and therefore cluster as within-sample

- **Mixed predictive distribution** for new units in *new* cluster:

$$\mathsf{E}_{\boldsymbol{\omega},\boldsymbol{\psi}|\boldsymbol{y}} f_{\mathsf{m}}(\boldsymbol{y}^{\mathsf{r}}_{j}|\boldsymbol{\omega},\boldsymbol{\psi}) = \int \underbrace{\left[\int f_{\mathsf{c}}(\boldsymbol{y}^{\mathsf{r}}_{j}|\boldsymbol{\omega},\boldsymbol{\zeta}_j) g(\boldsymbol{\zeta}_j|\boldsymbol{\psi})d\boldsymbol{\zeta}_j\right]}_{f_{\mathsf{m}}(\boldsymbol{y}^{\mathsf{r}}_{j}|\boldsymbol{\omega},\boldsymbol{\psi})} p(\boldsymbol{\omega},\boldsymbol{\psi}|\boldsymbol{y})d\boldsymbol{\omega}d\boldsymbol{\psi}$$

  Uses **prior** for $\boldsymbol{\zeta}_j$
  $\Rightarrow$ treats ζ_j and therefore cluster as out-of-sample

[Gelman, Meng & Stern, 1996]

Conditional WAIC and LOuO-CV

$$\mathsf{WAIC_c} = -2\sum_{j=1}^{J}\sum_{i=1}^{n_j}\log\left[\mathsf{E}_{\boldsymbol{\omega},\zeta_j|\boldsymbol{y}} f_{\mathsf{c}}(y_{ij}|\boldsymbol{\omega},\zeta_j)\right] + 2p_{\mathsf{Wc}}$$

$$p_{\mathsf{Wc}} = \sum_{j=1}^{J}\sum_{i=1}^{n_j}\mathsf{Var}_{\boldsymbol{\omega},\zeta_j|\boldsymbol{y}}\left[\log f_{\mathsf{c}}(y_{ij}|\boldsymbol{\omega},\zeta_j)\right]$$

- Same target as leave-one-unit out (LOuO) CV

$$-2\,\mathsf{LOuO\text{-}CV} = -2\sum_{j=1}^{J}\sum_{i=1}^{n_j}\log\mathsf{E}_{\boldsymbol{\omega},\zeta_j|\boldsymbol{y}_{-ij}} f_{\mathsf{c}}(y_{ij}|\boldsymbol{\omega},\zeta_j)$$

Conditional WAIC and LOuO-CV

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- $\mathsf{WAIC_c}$ and PSIS-LOuO provided by combination of `Stan` and R package `loo` [Vehtari, Gelman & Gabry, 2016]

Marginal WAIC and LOcO-CV

$$
\begin{aligned}
\mathsf{WAIC_m} &= -2\sum_{j=1}^{J} \log\left[\mathsf{E}_{\boldsymbol{\omega},\boldsymbol{\psi}|\boldsymbol{y}} f_{\mathsf{m}}(\boldsymbol{y}_j|\boldsymbol{\omega},\boldsymbol{\psi})\right] + 2p_{\mathsf{Wm}} \\
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  - Used for unclustered data with latent variables (e.g., overdispersed Poisson, meta-analysis) [Li, Qui & Feng, 2016; Millar, 2018]

WAIC and LOO-CV for unclustered data

- In unclustered data with **univariate** y_j (instead of $\boldsymbol{y}_j$), posterior predictive density collapses to mixed predictive density

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- Therefore conditional PSIS-LOO makes no sense and not clear what WAIC_{c} represents!

[Millar, 2018]

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- $\mathrm{WAIC_m}$ much better approximation to LOO-CV
  Also found in other applications [Li, Qui & Feng, 2016; Millar, 2018]

Dan Furr: Application to IRT

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- Web page on Education Research using Stan: `https://education-stan.github.io` (contributions welcome)
  - Tutorial and case-studies on IRT
  - Papers that use Stan in education research, broadly construed