Structured variable selection with continuous shrinkage priors

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Outline

Outline

Context

Dependence structures between variables may be induced by various factors in different applications:

- Between observations in the response variable:
    - Structure in space and/or time (Dynamic linear model, state-space model, spatio-temporal model,...)
    - Structure induced by grouping factors (Linear mixed model,...)
    - ...
- Between predictors:
    - Dependence structure between genes belonging to the same biological pathways or co-expressed (Gaussian graphical model,...),
    - Dependence structure between covariates collected over years,
    - ...

Such structures need to be taken into account into statistical models

Context

In many domains high-dimensional data are generated: the number of variables p may be greater than the number of observations n:

- Genetic/genomic studies: high-throughput technologies provide genetic/genomic information on the whole genome,
- Environmental studies: high-throughput technologies provide regular and intense monitoring of phenotypic traits over time,
- ..

Need to use statistical approaches preventing ill-posed problems (**non-invertible matrix**, **overfitting**) and leading to **parsimonious** models

Context

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    - ...
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Linear model context

$$Y = X\beta + \varepsilon,\ \varepsilon \sim \mathcal{N}_n(0, \sigma^2 I_n)$$

with

- $Y = (y_1, \ldots, y_n)'$ the n-vector of observations,
- X the $n \times p$ matrix of predictors which may be structured and/or of high dimension,
- $\beta = (\beta_1, \ldots, \beta_p)'$ the p-vector of coefficients,
- $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_n)'$ the n-vector of residuals,
- σ^2 the residual variance.

$\looparrowright$ To estimate parameters β and σ^2

Classical regression technique

Ordinary Least Square (OLS) regression

To minimize the lost function $L^{OLS}(\beta) = \| Y - X\beta \|^2$:

$$\hat{\beta}^{OLS} = (X'X)^{-1}(X'Y)$$

But

- In presence of structures between predictors (as collinearity): $(X'X)^{-1}$ close to singularity and so, $\hat{\beta}^{OLS}$ not accurate
- When the number of predictors is high: $\hat{\beta}^{OLS}$ does not perform well in unseen datasets (overfitting), does not provide parsimonious models (Hadamard, 1902) and in very high dimension $(X'X)^{-1}$ not invertible

↪ Need to use **regularization methods**

Regularization methods

Consist in introducing additional information into the problem:

- By imposing constraints as in ANOVA,
- By adding a penalty term to the minimization of the loss function as in **penalized regressions** (Ridge (Hoerl and Kennard, 1970), Lasso (Tibshirani, 1996),..),
- By specifying a dependence structure for effects of variables,
- ...

Bayesian approach: a natural framework

Bayesian approaches

In Bayesian framework additional information integrating into models via prior distributions

$\looparrowright$ Regularization is done by specifying **specific priors**

Selection

To shrink towards zero small coefficients while leaving large signals large: **Shrinkage** priors

Structure

Priors with a **variance-covariance matrix** related to structure information between variables

Objective:

To present **shrinkage** priors integrating **structure** information to select structured variables

Outline

Shrinkage priors

Two classes of shrinkage priors:

- **Spike-and-slab priors**: Discrete mixture of two distributions (Mitchell and Beauchamp, 1988; George and McCulloch, 1997)
- **Continuous shrinkage priors**: Unimodal continuous distributions (Bayesian Lasso prior, Horseshoe prior, Elastic-Net prior, ...) (Kyung et al., 2010; Carvalho et al., 2008)

Spike-and-slab prior

- Introduction of γ:

$$\gamma_j = \begin{cases} 1 \text{ if variable } j \text{ is selected} \\ 0 \quad \text{otherwise} \end{cases}$$

$$\beta_j|(\gamma_j = 1) \sim p_{Slab}(\beta_j)$$

$$\beta_j|(\gamma_j = 0) \sim p_{Spike}(\beta_j)$$

- The estimation of $\mathbb{P}(\gamma_j = 1|Y)$ gives access to the a posteriori probability of variable selection

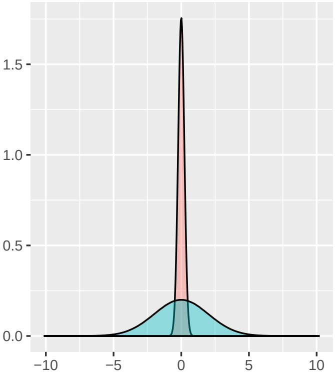


Figure 1: Spike-and-Slab prior distribution. Slab part in blue and spike part in red

Continuous shrinkage prior

Bayesian version of penalized approaches:

$$\beta_j | \tau^2, \omega_j \sim \mathcal{N}(0, \tau^2 \omega_j^2) \;\; j = 1, \ldots, p$$

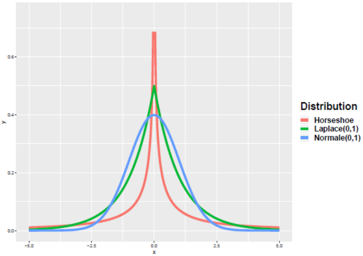
$$\tau^2, \omega_j^2 \sim \mathcal{F}(\tau^2; \omega_j^2)$$

where

- $\mathcal{F}$ is a distribution to specify

  $\looparrowright$ Bayesian Lasso prior, **Global-local priors**, ...

Figure 2: Continuous shrinkage prior distributions



Horseshoe prior (Carvalho et al., 2009)

A global-local prior with $\tau \sim \mathcal{C}^+(0,1)$ and $\omega_j \sim \mathcal{C}^+(0,1)$ $j = 1, \ldots, p$

- τ controls the global shrinkage
- ω_j controls the individual shrinkage: allows large signals to escape from the overall shrinkage

Outline

Structure

$$Y = X_1\beta_1 + \cdots + X_p\beta_p + \varepsilon,\ \varepsilon \sim \mathcal{N}_n(0, \sigma^2)$$

- X the $n \times p$ matrix of predictors which may be structured and/or of high dimension,

$\looparrowright$ $\beta = (\beta_1, \ldots, \beta_p)' \sim \mathcal{N}_p(0, \Sigma)$ with Σ related to structure between variables

$\looparrowright$ **Context dependent**

Examples

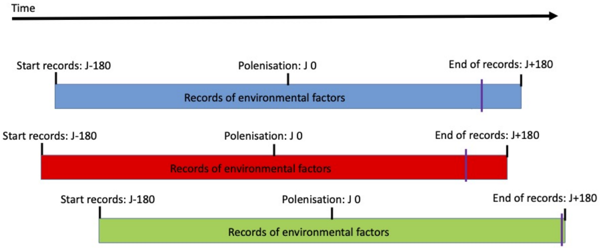
- $X_{t-1} \not\perp\!\!\!\perp X_t$: $\Sigma = AR(\rho)$ with ρ autoregressive parameter
- X_i's belong to a same group (pathways in genomic, genes in genetic, ...)

Outline

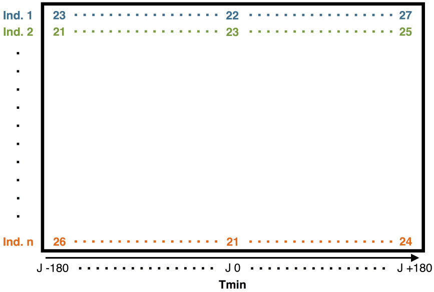
Biological motivation

Objective: to understand the impact of environmental variables on the process of fruit abscission in oil palm.
Dataset provided by "le Centre de Recherches Agricoles-Plantes Pérennes (CRA-PP)" (Tisné et al., 2020)

Oil palm: fruit abscission process

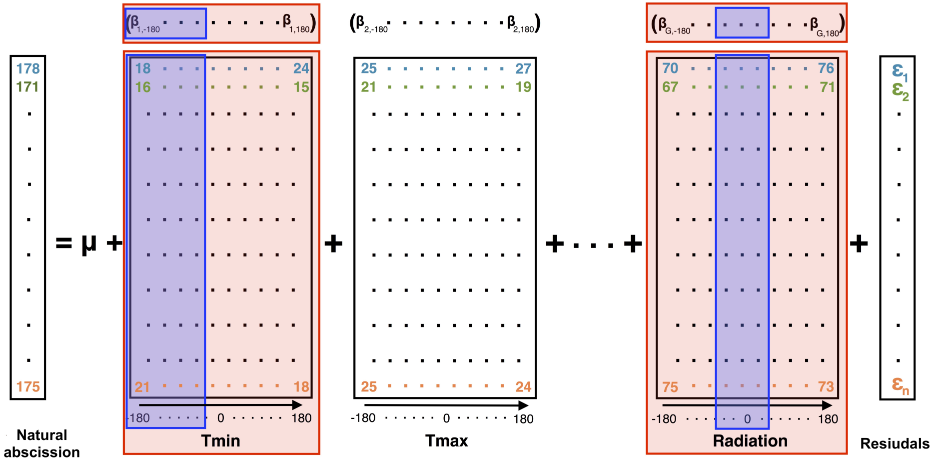


- **Climatic factors:**
  Temperature, rainfall, ...
- **Ecophysiological factors:**
  Evapotranspiration, photosynthesis, ...



Oil palm: fruit abscission process

To identify the environmental variables and the time periods affecting the oil palm fruit abscission process



Statistical questions

Linear model:

$$\boldsymbol{y} = \mu + \sum_{g=1}^{G} \boldsymbol{X_g} \boldsymbol{\beta_g} + \varepsilon,\ \varepsilon \sim \mathcal{N}_n(0, \sigma^2 I_n)$$

Selection:

- To identify environmental variables $\rightarrow$ Selection of grouped variables
  $\hookrightarrow$ Selection of grouped parameters: $(\beta_{g,-180}, \ldots, \beta_{g,180})' = (0, \ldots, 0)'$?
- To identify time periods $\rightarrow$ Selection of variables
  $\hookrightarrow$ Selection of parameters $\beta_{g,t} = 0$?

Double structure:

- Grouped variables
  $\looparrowright$ Integration of group structure
- Repeated measures over time for each environmental variables
  $\looparrowright$ High correlation between successive variables: to integrate natural order of variables on regression coefficients $\boldsymbol{\beta}_g = (\beta_{g,-180}, \ldots, \beta_{g,180})'$

Group fused horseshoe prior

To combine the horseshoe and the fused (Tibshirani et al., 2005) priors.

$$\boldsymbol{\beta_g} | \tau^2, \lambda_g^2, \boldsymbol{\omega_g^2}, \boldsymbol{\upsilon_g^2}, \sigma^2 \sim \mathcal{N}_T\left(0, \sigma^2 \left(\frac{\boldsymbol{D_g'}\boldsymbol{\Omega_g^{-1}}\boldsymbol{D_g}}{\tau^2\lambda_g^2} + \boldsymbol{\Upsilon_g^{-1}}\right)^{-1}\right)$$

$$\tau,\ \lambda_g,\ \omega_{g,t},\ \upsilon_{g,t} \sim \mathcal{C}^+(0,1)$$

1st matrix: to penalize differences while allowing abrupt changes

- τ^2: global hyperparameter
- λ_g^2: local hyperparameters specific to each group (environmental variables)
- $\omega_{g,t}^2$: local hyperparameter specific to difference $\beta_{g,t+1} - \beta_{g,t}$

2nd matrix: to add an additional level of penalization to shrink towards zero small effects

- $\upsilon_{g,t}^2$ local hyperparameter specific to the effect $\beta_{g,t}$

$\hookrightarrow$ Extension of priors: *sparse group horseshoe* (Xu et al., 2016), *fusion horseshoe* (Faulkner and Minin, 2018), *fused Laplace* (Kyung et al., 2010)

Inference: Gibbs algorithm (Markov chain Monte Carlo method). R code available at: https://github.com/Heuclin/GroupFusedHorseshoe

Simulation study

- Different profiles over time: smooth or with abrupt changes
- Comparisons with usual approaches:

↬ Sparse PLS, Elastic-net, Penalized regression with composite MCP penalty, Penalized regression with composite MCP + ridge

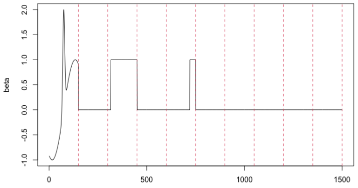


Figure 4: Simulated profiles for G=10 groups over T=150 time points

Results

- Group fused horseshoe outperforms other approaches in terms of selection, estimation, and prediction

↬ Robust: no sensitive to the ratio sample size / number of variables

↬ Stable: low variability between repetitions

Application on oil palm

Data

- 1,173 bunches (statistical unit)
- Outcome (y): number of days from pollination to fruit drop
- 5 climatic variables: Tmax, Tmin, Relative air humidity (RH), Rainfall (R), Solar radiation (SR)
- 5 ecophysiological variables: Maximum daily vapor pressure deficit (VPD), Fraction of transpirable soil water (FTSW), Supply-demand ratio (SD), Daily reproductive demand (DRD)
- 121 time points for each environmental variables: $p = 1,210$ predictors greater than $n = 1,173$ observations

Application on oil palm

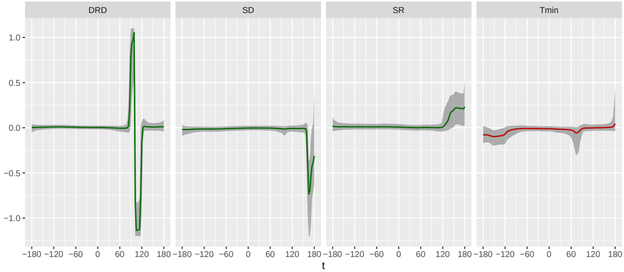


Figure 5: Estimated coefficient profiles for DRD, SD, SR, Tmin. Gray shadows represent the 95% credible interval.

- Identification of 4 environmental variables: DRD, SD, SR, Tmin
- Identification of relevant time periods
  - Tmin: smooth effect during the inflorescence development
  - DRD and SD: punctual effects at the end of the fruit bunch development
  - SR: smooth effect at the end of the fruit bunch development

Outline

Motivations

Most of the dependence structures between variables may be encoded by an undirected graph
↬ We propose to extend the approach proposed by Faulkner and Minin (2018); Faulkner (2019) to the more general context of graph-structured variables by combining:

1. The **efficiency and flexibility** of the horseshoe (HS) prior in terms of selection and estimation:
2. With a Gaussian Markov random field (GMRF) for its **appealing connection** with undirected graphs (Rue and Held, 2005):

↬ allows to impose the dependence structure between the parameters via the precision matrix of a conditionally Gaussian prior thus leading to sparse matrices and to smooth coefficients over the graph with possible abrupt changes

Bayesian hierarchical model

We assume that $\mathcal{G} = \bigcup_{i=1}^{I} \mathcal{G}_i = \bigcup_{i=1}^{I}(V_i, E_i)$ a disjoint union of I subgraphs and $\mathcal{S}$ the set of indices associated to one representative of each of the I subgraphs.

HS-GMRF model

$$
\begin{aligned}
\boldsymbol{y}|\boldsymbol{\beta}, \sigma^2 \quad &\sim \quad \mathcal{N}_n(\boldsymbol{X}\boldsymbol{\beta}, \sigma^2 \mathrm{I}_n) \\
\beta_j - s_{jj'}\beta_{j'}|\tau_{jj'}^2, \lambda^2 \quad &\sim \quad \mathcal{N}(0, \lambda^2\tau_{jj'}^2) \text{ for } (j, j') \in \bigcup_{i=1}^{I} E_i \\
\beta_j|\tau_j^2, \lambda^2 \quad &\sim \quad \mathcal{N}(0, \lambda^2\tau_j^2) \text{ for } j \in \mathcal{S} \\
\tau_{jj'} \quad &\sim \quad \mathcal{C}^+(0,1) \text{ for } (j, j') \in \bigcup_{i=1}^{I} E_i; \tau_j \sim \mathcal{C}^+(0,1) \text{ for } j \in \mathcal{S} \\
\lambda|\sigma \quad &\sim \quad \mathcal{C}^+(0,\sigma);\ \sigma^2 \sim \mathcal{IG}(a_0, b_0)
\end{aligned}
$$

with $s_{jj'} = \mathrm{sign}\{\mathrm{cor}(X_j, X_{j'})\}$ to encourage regression coefficients of negatively correlated variables to take opposite signs.

Simulation study

Objectives

- To evaluate the performances of the proposed approach with and without incorporating the sign of the sample correlation (HS-GMRF and HS-GMRF-nosign),
- To compare the results with two other approaches: the HS and the spike-and-slab with Ising prior (SS-Ising) (Smith and Fahrmeir, 2007; Li and Zhang, 2010) and when the true graph is known and unknown.

$Y = \sum_{g=1}^{G} \boldsymbol{X_g}\beta_g + \varepsilon$ with $X_{i,g} = (X_{i;g1}, \ldots, X_{i;gk})' \sim \mathcal{N}_k(0, \Sigma_g)$ and $\varepsilon \sim \mathcal{N}_n(0, \sigma^2 I_n)$

12 simulated scenarios

- Two covariance structures
- Two levels of correlation ($\rho = 0.5, 0.9$)
- Three regression coefficients

↬ Focus on the scenario where half of groups with Σ_g and

$$\beta_g = (5, -\tfrac{5}{\sqrt{10}}, -\tfrac{5}{\sqrt{10}}, \underbrace{\frac{5}{\sqrt{10}}, \ldots, \frac{5}{\sqrt{10}}}_{k-3})$$

Simulations

- $G = 14$ groups of $k = 10$ predictors,
- Only groups $g = 1, 3, 5, 8, 10$ have non-zero effects,
- $\sigma^2 = \sum_{g=1}^{G} \beta_g^2 / 5$
- Repetitions: 50

Simulation study

Performance criteria

- Variable selection criteria:
  ↬ For HS-based: variable selected if 95% HPD interval does not contain 0,
  ↬ For SS-Ising: variable selected if marginal inclusion posterior probabilitie greater than 0.5.
- Matthews correlation coefficient (MCC),
- Mean squared error (MSE) of the regression coefficients,
- Mean squared prediction error (MSPE).

Results

Table 1: Average MCC, MSE and MSPE (with SE) over 50 simulated replications.

		MCC	MSE	MSPE
$\Sigma_{g,\text{half}}$ $\rho = 0.5$	HS-GMRF	**0.708** ($\pm$ 0.018)	**0.513** ($\pm$ 0.067)	**94.871** ($\pm$ 13.632)
	HS-GMRF-nosign	0.624 ($\pm$ 0.034)	0.728 ($\pm$ 0.155)	122.188 ($\pm$ 21.609)
	HS	0.240 ($\pm$ 0.041)	1.009 ($\pm$ 0.200)	126.252 ($\pm$ 19.657)
	SS-Ising	0.323 ($\pm$ 0.054)	1.386 ($\pm$ 0.204)	149.294 ($\pm$ 27.384)
$\Sigma_{g,\text{half}}$ $\rho = 0.9$	HS-GMRF	**0.668** ($\pm$ 0.046)	**0.541** ($\pm$ 0.089)	**84.954** ($\pm$ 14.485)
	HS-GMRF-nosign	0.444 ($\pm$ 0.117)	1.038 ($\pm$ 0.259)	99.123 ($\pm$ 17.694)
	HS	0.219 ($\pm$ 0.038)	2.243 ($\pm$ 0.551)	95.219 ($\pm$ 19.279)
	SS-Ising	0.312 ($\pm$ 0.048)	2.359 ($\pm$ 0.437)	109.387 ($\pm$ 23.713)

- HS-GMRF-based approaches lead to the best results in terms of MCCs, MSEs, and MSPEs,
- HS-GMRF outperforms HS-GMRF-nosign especially when $\rho = 0.9$

Results

Table 2: Average MCC and MSE for connected and non-connected covariates over 50 simulated replications.

	MCC		MSE	
	Connected	Non-connected	Connected	Non-connected
	$\Sigma_{g,\text{half}}$ $\rho = 0.5$			
HS-GMRF	**0.956** ($\pm$ 0.033)	0.277 ($\pm$ 0.039)	**0.558** ($\pm$ 0.061)	**0.469** ($\pm$ 0.111)
HS-GMRF-nosign	0.810 ($\pm$ 0.053)	0.264 ($\pm$ 0.057)	0.913 ($\pm$ 0.202)	0.542 ($\pm$ 0.151)
HS	0.237 ($\pm$ 0.038)	0.244 ($\pm$ 0.054)	1.464 ($\pm$ 0.374)	0.553 ($\pm$ 0.139)
SS-Ising	0.332 ($\pm$ 0.062)	**0.295** ($\pm$ 0.096)	2.028 ($\pm$ 0.372)	0.744 ($\pm$ 0.208)
	$\Sigma_{g,\text{half}}$ $\rho = 0.9$			
HS-GMRF	**0.883** ($\pm$ 0.078)	0.278 ($\pm$ 0.049)	**0.611** ($\pm$ 0.138)	**0.470** ($\pm$ 0.091)
HS-GMRF-nosign	0.526 ($\pm$ 0.177)	0.265 ($\pm$ 0.053)	1.582 ($\pm$ 0.465)	0.495 ($\pm$ 0.112)
HS	0.188 ($\pm$ 0.043)	0.271 ($\pm$ 0.046)	3.998($\pm$ 1.105)	0.488 ($\pm$ 0.103)
SS-Ising	0.310 ($\pm$ 0.047)	**0.304** ($\pm$ 0.081)	4.055 ($\pm$ 0.855)	0.662 ($\pm$ 0.135)

- Performances for non-connected predictors are similar for HS and HS-GMRF-based approaches.
- For connected variables the integration of the dependence structure helps to select variables with small effects

Results

Table 3: Coverage probability (CP) and width of 95% HPD intervals averaged over the 50 simulated replications.

			CP of 95% HPD	Width of 95% HPD
$\Sigma_{g,\mathrm{half}}$	$\rho = 0.5$	HS-GMRF	0.923 ($\pm$0.026)	2.047 ($\pm$0.188)
		HS-GMRF nosign	0.931 ($\pm$0.027)	2.712 ($\pm$0.231)
		HS	0.894 ($\pm$0.037)	2.871 ($\pm$0.278)
		SS-Ising	0.751 ($\pm$0.026)	0.656 ($\pm$0.117)
	$\rho = 0.9$	HS-GMRF	0.928 ($\pm$0.019)	2.415 ($\pm$0.248)
		HS-GMRF nosign	0.922 ($\pm$0.031)	3.212 ($\pm$0.284)
		HS	0.908 ($\pm$0.05)	3.255 ($\pm$0.419)
		SS-Ising	0.773 ($\pm$0.029)	0.927 ($\pm$0.181)

- CPs similar for HS-based approaches but wider intervals for HS

Results

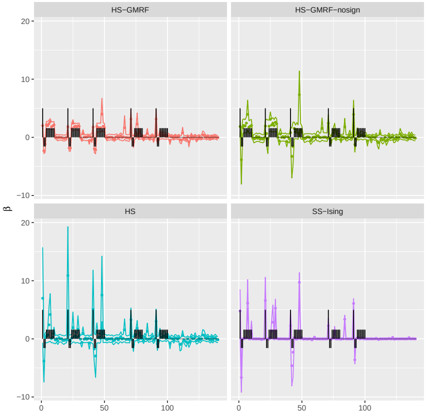


Figure 6: Estimated coefficients along with 80% HPD intervals in one simulated replication ($\Sigma_{g,\text{half}}$, $\rho = 0.9$).

- HS and SS-Ising tend to select one representative of a group of correlated variables,
- HS gives wide HPD intervals,
- HS-GMRF-based approaches give similar estimates for highly correlated covariates,
- HS-GMRF yields narrower HPD intervals with good coverage and fairly accurate estimates for regression coefficients with opposite signs.

Outline

Conclusion/Perspectives

Conclusion

Two priors proposed to select structured variables:

- Efficient combination and extension of existing approaches to deal with high-dimensional structured predictors,
- Flexibility and efficiency of horseshoe prior, via the local and global shrinkage hyperparameters, to handle different structures and to select relevant variables and/or groups of variables,
- Encompass a broad type of dependence structures : applicable in various applications (varying coefficient models, near infrared spectroscopy context (NIRS), QTL mapping, ...)

Perspectives

- To integrate prior knowledge on strengths of connections,
- To integrate dependence structures between observations,
- To extend to multivariate case (Y multivariate),
- To consider a multi-dimensional indexation.

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1. Introduction
   - Context
   - Selection
   - Structure
2. Group fused horseshoe prior
3. Horseshoe Gaussian Markov field prior
4. Conclusion/Perspectives
5. Bibliography

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