

# On Bayesian nonparametric regression

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2. bridging parametric & nonparametric  
Bayesian nonparametrics somehow extends parametric constructions to processes..
3. explosion of methods for **Bayesian nonparametric regression**.

However:

- still, less theory than for density estimation
- rich but fragmented literature
- little “ready-to-go” software

→ aim: a brief overview, having these issues in mind

Regression is possibly the most important problem in Statistics

Classical approaches now 'compete' with machine learning methods, deep learning, and more....

more bridges?

frequentist/Bayesian; ... parametric/nonparametric, ...  
*statistics/machine learning? ... probabilistic/non-probabilistic?*

Anyway, the basic issue of **quantifying the uncertainty** remains crucial. The output of regression is the basis for risk evaluation and decision. A poor quantification of uncertainty may be a disaster...

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Anyway, the basic issue of **quantifying the uncertainty** remains crucial. The output of regression is the basis for risk evaluation and decision. A poor quantification of uncertainty may be a disaster...

..and the Bayesian approach is based on quantifying information and uncertainty!

## Bayesian Deep Learning

NIPS 2016 Workshop

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Abstract

Schedule & Accepted Papers

Topics

Call for papers

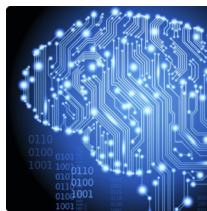
Travel Awards

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### Abstract

While deep learning has been revolutionary for machine learning, most modern deep learning models cannot represent their uncertainty nor take advantage of the well studied tools of probability theory. This has started to change following recent developments of tools and techniques combining Bayesian approaches with deep learning. The intersection of the two fields has received great interest from the community over the past few years, with the introduction of new deep learning models that take advantage of Bayesian techniques, as well as Bayesian models that incorporate deep learning elements [1-11].

In fact, the use of Bayesian techniques in deep learning can be traced back to the 1990s, in seminal works by Radford Neal [12],



### Bayesian nonparametrics

$$X_i | F \stackrel{iid}{\sim} F, \quad F \sim \text{prior distribution.}$$

The most popular *nonparametric* prior, the Dirichlet process, is the extension to a process of the Dirichlet conjugate prior for (*parametric*) multinomial sampling.



## motivation - 2. parametric conjugate priors

$X | \xi \sim p(x | \xi)$  in the NEF,

$\xi \sim$  **standard conjugate prior** (Diaconis & Ylvisaker, 1979).

Bernoulli	Beta
Multinomial	Dirichlet
$N(0, \Sigma)$	Inverse-Wishart
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But, conjugate priors for a **multivariate** NEF are restrictive.

Generalized Dirichlet	Connor & Mosiman (1969)
Generalized Wishart	Brown, Le, Zidek (1994)
<b>Enriched conjugate priors</b>	Consonni and Veronese (2001)
$\vdots$	$\vdots$

If  $f(x_1, \dots, x_k; \xi)$  NEF, and can be decomposed in a product of NEF densities, each having its own parameters, the **enriched conjugate prior on  $\xi$**  is obtained by giving a standard conjugate prior for each of those densities.

- $(X, Y) \mid \Sigma \sim N_k(0, \Sigma)$ .  
decompose  $f(x, y; \Sigma) = f_x(x; \phi)f(y \mid x; \theta)$  (both Gaussian),  
and assign conjugate priors of  $\phi$  and  $\theta$ .  
→ **Generalized Wishart** on  $\Sigma^{-1}$ .
- $(N_1, \dots, N_k) \mid (p_1, \dots, p_k) \sim \text{Multinomial}(N, p_1, \dots, p_k)$ .  
Re-write the multinomial as a product, by suitable  
reparametrization  
→ **Generalized Dirichlet distribution** for  $(p_1, \dots, p_k)$ .

The DP extends to a process. Let  $X_i | F \stackrel{iid}{\sim} F$ .

A Dirichlet process prior for  $F$ ,  $F \sim DP(\alpha F_0)$ , is such that, for any finite partition, the random vector of probabilities

$$(p_1, \dots, p_k) = (F(A_1), \dots, F(A_k)) \sim \text{Dir}(\alpha F_0(A_1), \dots, \alpha F_0(A_k))$$

(Ferguson, 1973).

The DP inherits **conjugacy** from the conjugacy of the Dirichlet distribution for multinomial sampling; but also its **lack of flexibility**. This is the more true when  $F$  is on  $\mathfrak{R}^k$ .

...An enriched conjugate **nonparametric** prior?

Doksum's Neutral to the Right Process (Doksum, 1974) extends the enriched conjugate Dirichlet distribution to a process.

# Enriched conjugate prior distributions: non-parametric

Doksum's Neutral to the Right Process (Doksum, 1974) extends the enriched conjugate Dirichlet distribution to a process.

However, NTR processes are limited to **univariate** random distributions.

The Dirichlet distribution implies that **any permutation** of  $(p_1, \dots, p_k)$  is completely neutral (that is,  $p_1, p_2/(1 - p_1), \dots, p_k/(1 - \sum_{j=1}^{k-1} p_j)$  are independent).

The Generalized Dirichlet only assumes that **one ordered vector**  $(p_1, \dots, p_k)$  is completely neutral. **In  $\mathfrak{R}$** , there is a natural ordering. **In more dimensions** (e.g., contingency tables  $p(x, y)$ ), there is no natural ordering.

(Wade, Mongelluzzo, P., 2011).

**Finite case:** we define an Enriched Dirichlet distribution for  $[p(x, y)]$  by choosing the ordering through  $p(x, y) = p_{y|x}(y | x)p_x(x)$ , and assuming that the vectors of the marginal and conditional probabilities have independent Dirichlet distributions.



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**Nonparametric case:**  $P(x, y)$  random distribution on  $\mathfrak{R}^k$ . Assume:

- $P_x \sim DP(\alpha_x P_{0,x})$
- for any  $x$ ,  $P_{y|x} \sim DP(\alpha_y(x) P_{0,y|x})$

all independent.

This well defines a probability law for the random  $P(x, y)$ , named **Enriched Dirichlet Process** (EDP)

## motivation - 3. Bayesian nonparametric regression

Focus on **mixture models** for

1. **conditional density estimation**: estimate  $f(y | x)$ , and
2. **density regression**: how the density  $f_x(y)$  of  $Y$  varies with  $x$ .

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- ① Details of the 'nonparametric' prior matter – not only for asymptotics, but for **finite sample prediction**.

We show the case of two different BNP priors, both consistent: but one of them is clearly *better* – **better exploits information**.

**Bayesian criteria to formalize such improvement?**

- ② Explosion of dependent Dirichlet processes (DDP) models. **How can we compare?** and offer a 'default choice' to practitioners, possibly in an **R-package?**

- 1 Preliminaries on BNP regression
- 2 Random design: DP mixtures for  $f(x, y)$ 
  - Example: Improving prediction by Enriched DP mixtures
- 3 Fixed design: Dependent stick-breaking mixture models
- 4 discussion

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# Density regression

$X$  predictor,  $p$ -dimensional;  $Y$  response.

\* Bayesian nonparametric (mean) regression:

$$: x \rightarrow m(x) = E(Y | x)$$

flexible model/prior on  $m(x)$  (basis expansions, Gaussian processes and splines (Wahba (1990), Denison, Holmes, Mallick, Smith (2002)), wavelets (Vidakovic, 2009), neural networks (Neal, 1996),...

\* Yet, the mean may be a too poor summary of the relationship between  $x$  and  $y$ .

$\Rightarrow$  median, quantile regression,.. density regression

$$: x \rightarrow f(y | x)$$

Limited literature on optimal estimators of  $f(y | x)$ . (Efromovich, Ann. Stat. 2007). How about Bayesian methods?

# Random or fixed design

- regression: random design

$(X_i, Y_i), i = 1, \dots, n$  are a random sample from  $f(x, y)$ .

Then, estimate the joint density  $f(x, y)$  and from this the conditional  $f(y | x) = \frac{f(x, y)}{f_x(x)}$ .

- fixed design

$x_1, \dots, x_n$  is a deterministic sequence. If predictor is  $x$ ,  $Y \sim f(y | x)$ . in fact,  $f_x(y)$ .

- replicates of  $y$  values at a given  $x$  ( $x$  typically categorical or ordinal), (e.g. ANOVA)
- no replicates ( $x$  typically continuous)  
still interest in  $f_x(y)$ : borrowing strength through smoothness conditions along  $x$ .

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## Random design: DP mixtures for $f(x, y)$

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\* Model  $f$  as a mixture of kernels:

$$\begin{aligned} (X_i, Y_i) \mid G &\stackrel{iid}{\sim} f_G(x, y) = \int K(x, y \mid \theta) dG(\theta) \\ G &\sim DP(\alpha G_0) \end{aligned}$$

Usually,  $K(x, y \mid \theta) = N_{p+1}(x, y \mid \mu, \Sigma)$ , with  $\theta = (\mu, \Sigma)$ , and  $G_0(\theta)$  conjugate prior.

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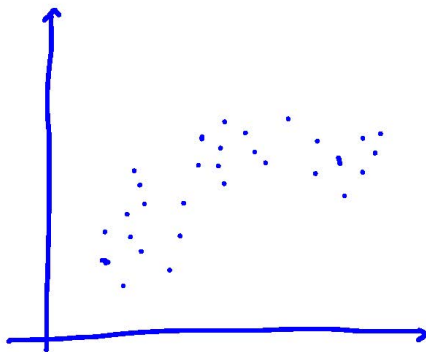
Usually,  $K(x, y \mid \theta) = N_{p+1}(x, y \mid \mu, \Sigma)$ , with  $\theta = (\mu, \Sigma)$ , and  $G_0(\theta)$  conjugate prior.

Since, a.s.,  $G = \sum_{j=1}^{\infty} p_j \delta_{\theta_j^*}$ , where  $(p_j) \sim \text{stick-breaking}(\alpha)$  independent of  $\theta_j^* \stackrel{iid}{\sim} G_0$ , the mixture above reduces to

$$f_G(x, y) = \sum_{j=1}^{\infty} w_j K(x, y \mid \theta_j^*).$$

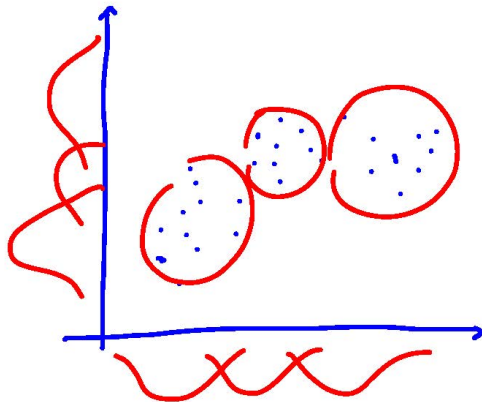
# mixture of Gaussian kernels

in picture



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# Latent variable representation

The DP-mixture model is equivalently expressed as

$$\begin{aligned}(X_i, Y_i) | \theta_i &\stackrel{ind}{\sim} K(x, y | \theta_i) \\ \theta_i | G &\stackrel{iid}{\sim} G \\ G &\sim DP(\alpha G_0)\end{aligned}$$

Integrating the  $\theta_i$  out, one has back the countable mixture model

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$$(X_i, Y_i) | G \stackrel{iid}{\sim} f_G(x, y) = \sum_{j=1}^{\infty} p_j K(x, y | \theta_j^*).$$

Then the conditional density  $f(y | x)$  is obtained as

$$f_G(y | x) = \frac{\sum_j p_j K(x, y | \theta_j^*)}{\sum_j p_j K(x | \theta_j^*)} = \sum_j p_j(x) K(y | x, \theta_j^*)$$

where  $p_j(x) = p_j K(x | \theta_j^*) / (\sum_{j'} p_{j'} K(x | \theta_{j'}^*))$ .

# Random partition

Since  $G$  is a.s. discrete, ties in a sample  $(\theta_1, \dots, \theta_n)$  from  $G$  have positive probability, so that

$(\theta_1, \dots, \theta_n)$  described by  $(\rho_n; \theta_1^*, \dots, \theta_{k(\rho_n)}^*)$

- a random partition  $\rho_n = (s_1, \dots, s_n)$
- the cluster-specific parameters  $\theta_j^*$

**Ex:** for  $n = 5$ ,  $\rho_n = (1, 1, 2, 2, 1)$  gives  $(\theta_1, \dots, \theta_n) = (\theta_1^*, \theta_1^*, \theta_2^*, \theta_2^*, \theta_1^*)$ ,  $k_n = 2$  two clusters of size  $n_1 = 3$ ,  $n_2 = 2$  resp., with cluster-specific parameters  $\theta_1^*, \theta_2^*$ .

- The DP induces a probability law of the random partition

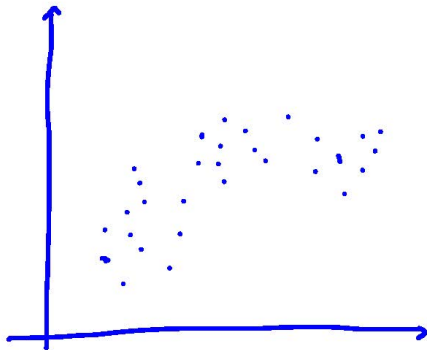
$$p(\rho_n) = \frac{\Gamma(\alpha)}{\Gamma(\alpha + n)} \alpha^{k_n} \prod_{j=1}^{k_n} \Gamma(n_j)$$

- Given the partition  $\rho_n$ , the cluster specific parameters  $\theta_j^*$  are i.i.d.  $\sim G_0$ .



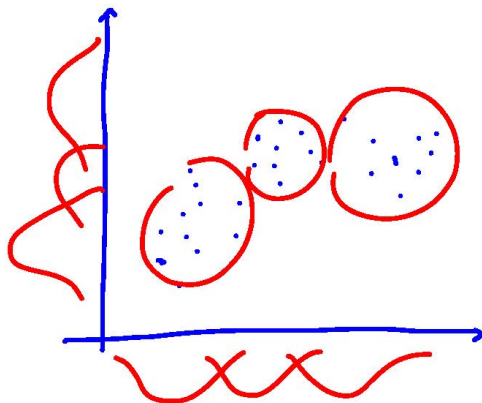
# mixture of Gaussian kernels

in picture

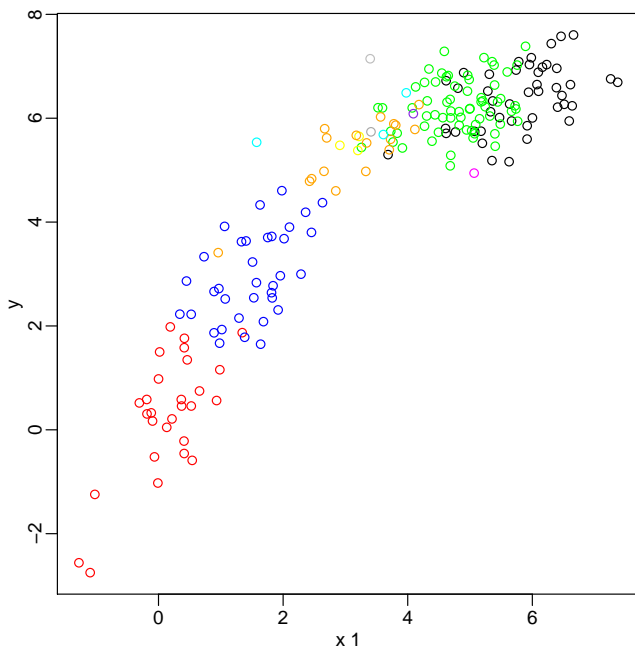


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\* **posterior on  $\rho_n$**

$$\begin{aligned}
 p(\rho_n \mid x_{1:n}, y_{1:n}) &\propto p(\rho_n) \prod_{j=1}^{k_n} \int \prod_{i:(x_i, y_i) \in S_j} K(x_i, y_i \mid \theta_j^*) dP_0(\theta_j^*) \\
 &\propto p(\rho_n) \prod_{j=1}^{k_n} m(\{(x_i, y_i) \in C_j\} \mid \rho_n)
 \end{aligned}$$

prior  $\times$  independent marginal likelihoods in each clusters.

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prior  $\times$  independent marginal likelihoods in each clusters.

\* **posterior on  $(\theta_j^*)$**  Given the partition, clusters are independent, and inference on  $\theta_j^*$  is based only on obs. in group  $C_j$

$$p(\theta_1^*, \dots, \theta_{k_n}^* \mid x_{1:n}, y_{1:n}, \rho_n) = \prod_{j=1}^{k_n} p(\theta_j^* \mid \rho_n, \{(x_i, y_i) \in C_j\})$$

# Predictive distribution (density estimate)

With quadratic loss, the Bayesian density estimate is the predictive density

$$(X_{n+1}, Y_{n+1}) \mid x_{1:n}, y_{1:n} \sim \hat{f}(x, y) = \mathbb{E}(f(x, y) \mid x_{1:n}, y_{1:n}).$$

\* Recalling that  $G \mid \theta_{1:n}, x_{1:n}, y_{1:n} \sim DP(\alpha G_0 + \sum_{i=1}^n \delta_{\theta_i})$ ,

$$\begin{aligned} \hat{f}(x, y) &= \mathbb{E}(\mathbb{E}(f_G(x, y) \mid \theta_{1:n}) \mid x_{1:n}, y_{1:n}) \\ &= \frac{\alpha}{\alpha + n} f_{G_0}(x, y) + \frac{n}{\alpha + n} \mathbb{E} \left( \sum_{i=1}^n \frac{K(x, y \mid \theta_i)}{n} \mid x_{1:n}, y_{1:n} \right) \end{aligned}$$

average of prior guess  $f_{G_0}$  and expectation of a **kernel estimate** with kernels centered at the  $\theta_j$ .

\* Since  $(\theta_1, \dots, \theta_n) \leftrightarrow (\rho_n, \theta_1^*, \dots, \theta_k^*)$ , the joint density estimate is

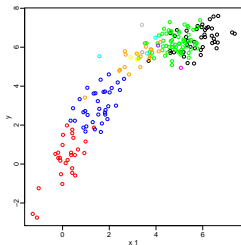
$$\hat{f}(x, y) = \frac{\alpha}{\alpha + n} f_{G_0}(x, y) + \sum_{\rho_n} \left( \sum_{j=1}^{k(\rho_n)} \frac{n_j(\rho_n)}{\alpha + n} f(x, y \mid (x_i, y_i) \in C_j(\rho_n)) \right) p(\rho_n \mid x_{1:n}, y_{1:n})$$

average of the prior guess  $f_{G_0}$ , and given the partition  $\rho_n$ , of the predictive densities in clusters  $C_j(\rho_n)$ .

From  $\hat{f}(x, y)$ , one can find an estimate of  $f(y \mid x)$ .

## 'clustering' and density estimate

The partition is not of main interest (mixture components just play the role of kernels), but  $p(\rho_n \mid x_{1:n}, y_{1:n})$  plays a crucial role.



Such role of the prior and posterior distribution of the random partition is often overlooked.



# How comparing nonparametric priors?

## Frequentist properties.

Results on frequentist asymptotic properties for multivariate density estimation, and some results for regression and conditional density estimation (Wu & Ghosal (2008; 2010); Tokdar (2011), Norets & Pelenis (2012), Shen, Tokdar & Ghosal (2013), Canale & Dunson (2015), Bhattacharya, Pati, Dunson (2014)– anisotropic; Norets & Pati (2016+), ...

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Different nonparametric priors may be consistent, but have quite diverse predictive performance!

The implied distribution on the random partition plays a crucial role.

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**Example 1.** Wade, Walker & Petrone (*Scand. J. Statist.*, 2014) introduce a **restricted partition model** to overcome difficulties of DP mixtures in curve fitting. Their proposal clearly leads to improved prediction.

## Problem: anisotropic case

$X$  continuous predictors; Gaussian kernels.

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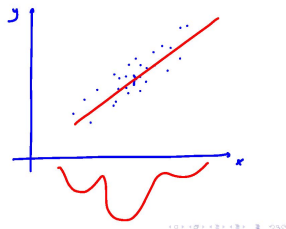
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in picture



here, many small clusters (kernels) are needed to fit the  $f_x$  density, while much fewer kernels would suffice for  $f_{y|x}$ .

If the dimension of  $x$  is large, the likelihood is dominated by the  $x$  component and many small clusters are suggested by the posterior on  $\rho_n$ . This impoverishes the performance of the model.

This undesirable behavior does not seem to vanish with increasing sample size.

If  $f_x(x)$  requires many clusters, the unappealing behaviour of the random partition could be reflected in worse convergence rates. Efromovich [2007] shows that if the conditional density is smoother than the joint, it can be estimated at a faster rate.

Thus, improving inference on the random partition to take into account the different degree of smoothness of  $f_x$  and  $f_{y|x}$  is crucial.

Consider the Dirichlet mixture of Gaussian kernels

$$(X_i, Y_i) \mid G \sim \int N_{p+1}(\mu, \Sigma) dG(\mu, \Sigma), \quad G \sim DP(\alpha G_0).$$

The base measure of the DP,  $G_0(\mu, \Sigma)$ , is usually Normal-Inv Wishart. **BUT, this conjugate prior is restrictive if  $p$  is large**



# Improving prediction

- Write the kernels as

$$N_{p+1}(x, y | \mu, \Sigma) = N_p(x | \mu_x, \Sigma_x) N(y | x' \beta, \sigma_{y|x}^2)$$

and use simple spherical  $x$ -kernels (Shahbaba and Neal, 2009, Hannah et al., 2011). Thus,

$$f_x(x | P) = \sum_{j=1}^{\infty} w_j N_p(x | \mu_{xj}^*, \begin{pmatrix} \sigma_{x1,j}^{2*} & 0 & \cdots & 0 \\ 0 & \sigma_{x2,j}^{2*} & 0 & 0 \\ 0 & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \sigma_{xp,j}^{2*} \end{pmatrix})$$

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$$f(y | x, P) = \sum_{j=1}^{\infty} w_j(x) N(y | x' \beta_j^*, \sigma_{y|x,j}^{2*}).$$

- Denote the  $x$ -parameters  $\phi = ((\mu_{x1}, \dots, \mu_{xp}), (\sigma_{x1}^2, \dots, \sigma_{xp}^2))$  and the  $y|x$ -parameters  $\theta = (\beta, \sigma_{y|x}^2)$ . Assign independent conjugate priors  $G_{0,\phi}(\phi)$  and  $G_{0,\theta}(\theta)$  (that leads to an enriched conjugate prior for  $(\mu, \Sigma)$ )

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$$N_{p+1}(x, y \mid \mu, \Sigma) = N_p(x \mid \mu_x, \Sigma_x) N(y \mid x' \beta, \sigma_{y|x}^2)$$

and use simple spherical  $x$ -kernels (Shahbaba and Neal, 2009, Hannah et al., 2011). Thus,

$$f_x(x \mid P) = \sum_{j=1}^{\infty} w_j N_p(x \mid \mu_{xj}^*, \begin{pmatrix} \sigma_{x1,j}^{2*} & 0 & \cdots & 0 \\ 0 & \sigma_{x2,j}^{2*} & 0 & 0 \\ 0 & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \sigma_{xp,j}^{2*} \end{pmatrix})$$

$$f(y \mid x, P) = \sum_{j=1}^{\infty} w_j(x) N(y \mid x' \beta_j^*, \sigma_{y|x,j}^{2*}).$$

- Denote the  $x$ -parameters  $\phi = ((\mu_{x1}, \dots, \mu_{xp}), (\sigma_{x1}^2, \dots, \sigma_{xp}^2))$  and the  $y|x$ -parameters  $\theta = (\beta, \sigma_{y|x}^2)$ . Assign independent conjugate priors  $G_{0,\phi}(\phi)$  and  $G_{0,\theta}(\theta)$  (that leads to an enriched conjugate prior for  $(\mu, \Sigma)$ )
- In the DP mixture model, assume individual-specific  $(\phi_i, \theta_i)$  as a random sample from  $G \sim DP(\alpha G_{0,\phi} G_{0,\theta})$

# Joint DP mixture model

$$\begin{aligned} Y_i | x_i, \beta_i, \sigma_{y,i}^2 &\stackrel{\text{ind}}{\sim} N(\beta_i' x_i, \sigma_{y,i}^2), \quad \theta_i = (\beta_i, \sigma_{y,i}^2), \\ X_i | \mu_i, \sigma_{x,i}^2 &\stackrel{\text{ind}}{\sim} \prod_{h=1}^p N(\mu_{x,h,i}, \sigma_{x,h,i}^2), \quad \phi_i = (\mu_{x,i}, \sigma_{x,i}^2) \\ (\theta_i, \phi_i) | G &\stackrel{\text{i.i.d.}}{\sim} G, \\ \mathbf{G} &\sim DP(\alpha G_{0\theta} \times G_{0\phi}). \end{aligned}$$

with  $G_{0\theta}$  and  $G_{0\phi}$  independent conjugate Normal-Inverse Gamma priors.

The model is flexible, and MCMC computations are standard.

BUT, if  $p$  is large, many (independent) kernels will be typically needed to describe the (dependent) marginal  $f_x$ , while the relationship  $Y | x$  can be smoother.

However, the DP only allows joint clusters of  $(\phi_i, \theta_i)$ ,  $i = 1, \dots, n$ .

Given its crucial role, difficulties in the random partition have relevant consequences on prediction

We would like to use a prior on  $P$  that allows many  $\phi_i$  clusters, to fit  $f_x$ , but fewer  $\theta_j$  clusters, and it is still conjugate, so that computations remain simple.

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⇒ Enriched Dirichlet Process (Wade, Mongelluzzo, P., 2011)

# Enriched Dirichlet Process

Extends the idea that leads from the Dirichlet distribution (conjugate to the multinomial) to the enriched (or generalized) Dirichlet dist. (Connor & Mosiman (1969);

and from the DP to Doksum (1974) neutral-to-the-right priors for random probability measures **on the real line**.

**EDP**: Assign a prior for the random prob. measure  $G(\theta, \phi)$  by assuming:

- $P_\theta \sim DP(\alpha_\theta P_{0,\theta})$
- for any  $\theta$ ,  $P_{\phi|\theta} \sim DP(\alpha_\phi(\theta) P_{0,\phi|\theta})$

all independent.

The EDP gives a **nested random partition**:  $\rho_n = (\rho_{n,\theta}, \rho_{n,\phi})$ , that **allows many  $\phi$ -clusters inside each  $\theta$ -cluster**.

## EDP: nested random partition

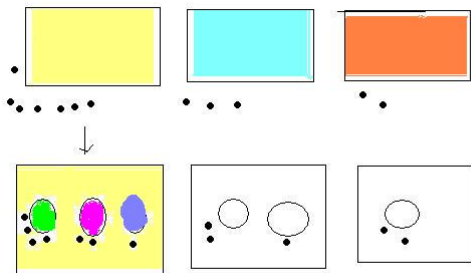
$\rho_n = (\rho_{n,\theta}, \rho_{n,\phi})$  : many  $\phi$ -clusters inside each  $\theta$ -cluster.



# EDP: nested random partition

$\rho_n = (\rho_{n,\theta}, \rho_{n,\phi})$  : many  $\phi$ -clusters inside each  $\theta$ -cluster.

- $P_\theta \sim DP(\alpha P_{0\theta})$  gives a Chinese restaurant process: customers choose *restaurants*, and restaurants are colored with colors  $\theta_h^* \stackrel{iid}{\sim} P_{0\theta}$  (nonatomic):
- $P_{\phi|\theta} \sim DP(\alpha_\phi(\theta) P_{0\phi|\theta})$  gives a *nested* CRP: within each restaurant, customers sits at tables as in the CRP. Tables in restaurant  $\theta_h^*$  are colored with colors  $\phi_{j|h}^* \stackrel{iid}{\sim} P_{0,\phi|\theta}(\phi | \theta)$ .



nested Chinese restaurant

- Model (replace DP with EDP):

$$Y_i | x_i, \beta_i, \sigma_{y,i}^2 \stackrel{\text{ind}}{\sim} N(\beta_i' x_i, \sigma_{y,i}^2), \quad \theta_i = (\beta_i, \sigma_{y,i}^2),$$

$$X_i | \mu_i, \sigma_{x,i}^2 \stackrel{\text{ind}}{\sim} \prod_{h=1}^P N(\mu_{x,h,i}, \sigma_{x,i,h}^2), \quad \phi_i = (\mu_{x,i}, \sigma_{x,i}^2)$$

$$(\theta_i, \phi_i) | \mathbf{G} \stackrel{\text{i.i.d.}}{\sim} \mathbf{G},$$

$$\mathbf{G} \sim \text{EDP}(\alpha_\theta, \alpha_\phi(\cdot), G_{0,\theta} \times G_{0,\phi|\theta}).$$

- Computations remain simple, as the EDP is a conjugate prior;
- Inference on a cluster-specific  $\theta_j^* = (\beta_j; \sigma_{y|x^*})$ , (thus, ultimately, on the conditional density  $f(y | x, \theta)$ ), exploits the information from the observations in all the  $\phi_h^*$ -clusters that share the same  $\theta_j^* \Rightarrow$  **much improved inference and prediction**

(Wade, Dunson, Petrone, Trippa, JMLR (2014))

# Simulation study

Toy example to demonstrate two key advantages of the EDP model

- it can **recover the true coarser  $\theta$ -partition**
- **improved prediction** and **smaller credible intervals** result.

Data: 200 obs  $(x_i, y_i)$  where

The covariates  $X_i$  are sampled from a  $p$ -variate normal,

$$X_i = (X_{i,1}, \dots, X_{i,p})' \stackrel{iid}{\sim} N(\mu, \Sigma),$$

centered at  $\mu = (4, \dots, 4)'$  with  $\Sigma_{h,h} = 4$  for  $h = 1, \dots, p$ , and covariances that model two groups of covariates with different correlation structure.

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The true regression only depends on the first covariate; it is a nonlinear regression obtained as a mixture

$$Y_i | x_i \stackrel{ind}{\sim} p(x_{i,1})N(y_i | \beta_{1,0} + \beta_{1,1}x_{i,1}, \sigma_1^2) + (1 - p(x_{i,1}))N(y_i | \beta_{2,0} + \beta_{2,1}x_{i,1}, \sigma_2^2)$$

Table: Prediction error for both models as  $p$  increases.

	$p = 1$		$p = 5$		$p = 10$		$p = 15$	
	$\hat{l}_1$	$\hat{l}_2$	$\hat{l}_1$	$\hat{l}_2$	$\hat{l}_1$	$\hat{l}_2$	$\hat{l}_1$	$\hat{l}_2$
DP	<b>0.03</b>	<b>0.05</b>	0.16	0.2	0.25	0.34	0.26	0.34
EDP	0.04	<b>0.05</b>	<b>0.06</b>	<b>0.1</b>	<b>0.09</b>	<b>0.16</b>	<b>0.12</b>	<b>0.21</b>

# Real data: Alzheimer disease diagnosis

Data were obtained from the [Alzheimer's Disease Neuroimaging Initiative \(ADNI\)](#) database, which is publicly accessible at UCLA's Laboratory of Neuroimaging.

**covariates:** summaries of  $p = 15$  brain structures computed from structural MRI obtained at the first visit for 377 patients, of which 159 have been diagnosed with AD and 218 are cognitively normal (CN).

**response:**  $Y_i = 1$  (cognitively normal subject); or  $= 0$  (diagnosed with AD).

**Aim:** Prediction of AD status

# Extension of the model to binary response

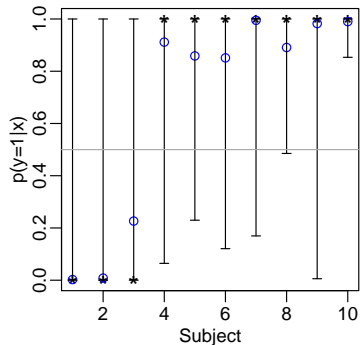
The model is extended to a local probit model:

$$Y_i | x_i, \beta_i \stackrel{iid}{\sim} \text{Bern}(\Phi(\underline{x}_i \beta_i)), \quad X_i | \mu_i, \sigma_i^2 \stackrel{iid}{\sim} \prod_{h=1}^p \text{N}(\mu_{i,h}, \sigma_{i,h}^2),$$
$$(\beta_i, \mu_i, \sigma_i^2) | G \stackrel{iid}{\sim} G, \quad \mathbf{G} \sim Q.$$

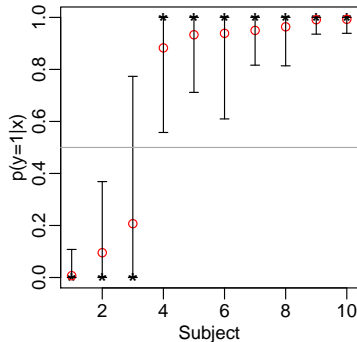
First, **DP prior for  $G$** :  $G \sim DP(\alpha, G_{0\beta} \times G_{0\psi})$ , with  $G_{0\beta} = \text{N}(0_p, C^{-1})$  and  $G_{0\psi}$  product of  $p$  normal-inverse gamma. We let  $\alpha \sim \text{Gamma}(1, 1)$ .

**EDP prior for  $G$** : correlation between the measurements of the brain structures and non-normal univariate histograms of the covariates suggest that many Gaussian kernels with local independence will be needed to approximate the density of  $X$ . The conditional density of the response, on the other hand, may not be so complicated. This motivates the choice of an EDP prior.

# Prediction for 10 new subjects



(a) DP



(b) EDP

**Figure:** Predicted probability of being healthy against subject index for 10 new subjects and represented with circles (DP in blue and EDP in red) with the true outcome as black stars. The bars about the prediction depict the 95% credible intervals.



- 1 Preliminaries on BNP regression
- 2 Random design: DP mixtures for  $f(x, y)$
- 3** Fixed design: Dependent stick-breaking mixture models
- 4 discussion

## Fixed design: Conditional models

Sample  $(x_i, Y_{i,\nu}), \nu = 1, \dots, n_i$ ,  $x$  fixed input.

Interest in  $f_x(y)$  (no longer a conditional  $f(y | x)$ ).

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Joint DP mixture models are used in this context, too. Yet, they unnecessarily require to model the marginal density  $f_x(x)$ .

In a Bayesian approach, one wants to assign a prior on the set of random prob. measures  $\{F_x(\cdot), x \in \mathcal{X}\}$ .

The random measures  $F_x$  must be dependent, as we want some smoothness along  $x$ , for borrowing strength; and have a given marginal distribution, e.g.  $F_x \sim DP$ .

Early proposals: Cifarelli & Regazzini (1978), extending mixtures of DP (Antoniak, 1974).

Influential idea: dependent Dirichlet processes (DDP), McEachern (1999; 2000), based on dependent stick-breaking constructions.

## DDP mixture models

Use a mixture model for  $f_x(y)$

$$Y_{i,\nu} | x, G_x \stackrel{ind}{\sim} f_{G_x}(y) = \int K(y | x, \theta) dG_x(\theta)$$

where the mixing distribution  $G_x$  is indexed by  $x$ .

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where the mixing distribution  $G_x$  is indexed by  $x$ .

A DDP prior on  $\{G_x, x \in \mathcal{X}\}$  assumes that  $G_x \sim DP(\alpha(x)G_{0,x})$ , and dependence is introduced through the dependent stick-breaking constructions:

$$G_x(\cdot) = \sum_{j=1}^{\infty} p_j(x) \delta_{\theta_j^*(x)}(\cdot)$$

where, for each  $j$ :

- $(w_j(x), x \in \mathcal{X})$  is a stochastic process, with stick-breaking construction  $w_1(x) = v_1(x)$ ;  $w_2(x) = v_2(x)(1 - v_1(x))$ , ... where  $(v_j(x), x \in \mathcal{X})$  is a stochastic process with marginals  $v_j(x) \sim \text{Beta}(1, \alpha(x))$ , and the  $v_j(\cdot)$  are independent across  $x$ ;
- $(\theta_j^*(x), x \in \mathcal{X})$  is a stochastic process with marginals  $G_{0,x}$ . The processes  $\theta_j(\cdot)$  are independent across  $j$ , and indep. of the  $v_j(\cdot)$ .

# Conditional approach: Single weights

The DDP allows both the mixing weights and the atoms to depend on  $x$ . But this is redundant, and one either considers 1) models with **single weights** and 2) models with **covariate dependent weights**.

**Single weights:** assume  $w_j(x) = w_j$  with flexible  $\theta_j(x)$ :

$$f_{G_x}(y|x) = \sum_{j=1}^{\infty} w_j K(y|\theta_j(x)).$$

- Ex.  $K(y|\theta_j(x)) = N(y|\mu_j(x), \sigma_j^2)$  with  $\mu_j \stackrel{iid}{\sim}$  GP.
- Popular because inference relies on established algorithms for BNP mixtures.

# Conditional approach: Covariate dependent weights

**Covariate dependent weights:** flexible  $w_j(x)$  with  $\theta_j(x) = \theta_j$ :

$$f_{P_x}(y|x) = \sum_{j=1}^{\infty} w_j(x) K(y|\theta_j, x),$$

for ex.  $K(y|\theta_j(x)) = N(y|\beta_j'x, \sigma_j^2)$ .

- Most techniques to define  $w_j(x)$  s.t.  $\sum_j w_j(x) = 1$  use a **stick-breaking approach**:

$$w_1(x) = v_1(x) \text{ and for } j > 1 \quad w_j(x) = v_j(x) \prod_{j' < j} (1 - v_{j'}(x)),$$

- Proposals for  $v_j(x)$  include Griffin and Steel (2006), Dunson and Park (2008), normalized weights model (Antoniano, Wade, Walker; 2014); probit stick-breaking (Rodriguez and Dunson, 2011); logit stick-breaking (Ren, Du, Carin & Dunson (2011); Rigon & Durante, 2017+), ...

How can we compare?



The EDP example shows clear improvement in the predictive performance. We would like to **formally express the gain of information** that a model/prior can provide.

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So far

- Careful and detailed study of the information and assumption introduced through the prior/model; and the analytic implications on the predictive distribution;
- compare on simulated and real data.

Some findings (Peruzzi, Petrone & Wade, 2016+)

- The 'single weights' mixture model needs flexible atoms, for giving reasonable prediction. But this has drawbacks, including identifiability.
- Covariate-dependent weights allow local selection of the clustering, and generally better prediction.

In particular, Peruzzi & Wade (2016+) compared the kernel stick-breaking model (Dunson & Park, 2008) and the normalized weights model (Antoniano, Wade, Walker, 2014). The latter appears to allow faster computations.

A substantial challenge for comparison is due to computations: one needs an algorithm that can give fast computations, and be fairly easily adapted to different models.

Peruzzi & Wade (2016+) suggest a clever algorithm, based on adaptive truncation and Metropolis-Hastings, moving from a proposal by Griffin (2016).

This is a necessary basis for providing R-packages for density regression and conditional density estimation.

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I tried to give an overview of proposals for Bayesian density regression, based on mixture models.

Careful study of the finite-sample properties of these models, for comparison

Together with flexible, easily-exportable computational tools, these are necessary steps for providing R-packages for density regression.

- Wade, S., Mongelluzzo, S. & Petrone, S. (2011). An enriched conjugate prior for Bayesian nonparametric inference. *Bayesian Analysis*, **3**, 359–386.
- Wade, S., Dunson, D., Petrone, S. & Trippa, L. (2014). Improving prediction from Dirichlet process mixtures via enrichment. *Journal of Machine Learning Research*, 1041–1071.
- Wade, S., Walker, S. & Petrone, S. (2014). A Predictive Study of Dirichlet Process Mixture Models for Curve Fitting. *Scandin. J. Statist.*, **41**, 580–605.
- Wade, S., Peruzzi, M. & Petrone, S. (2016+) Review of Bayesian nonparametric mixture models for regression. (*manuscript*)