Implicit Copulas from Bayesian Regularized Regression Smoothers

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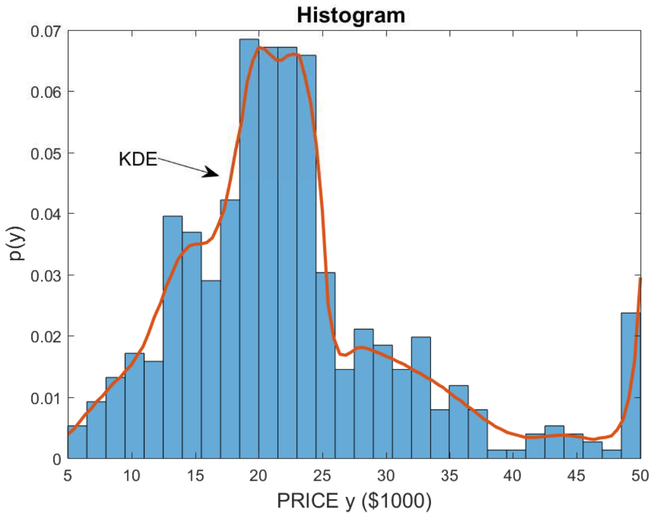
- Typical regression models relate the expectation of the response to covariates.
- ‘Statisticians are mean lovers’.
- This exclusive focus on the conditional expectation may however
  - possibly not meaningful and insufficient,
  - often not flexible enough,
  - does not comply to the main goal of the analysis.

Motivating Example: The Boston Housing Data

- Popular nonparametric regression dataset with $n = 506$ and
  - Y: Median house price in a census tract
  - covariates $\boldsymbol{X}$: NOX, RN, DIS, LSTAT, TAX
- Aim: Estimate a nonparametric regression model such that the entire distribution $F(Y|\boldsymbol{X})$ is a function of $\boldsymbol{X}$ and e.g.

$$E(Y|\boldsymbol{X}) = f(\boldsymbol{X}).$$

- However: The marginal distribution of Y is highly non-Gaussian


Histogram
KDE
p(y)
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
5
10
15
20
25
30
35
40
45
50
PRICE y ($1000)

Bayesian Distributional Regression

- Observed data pairs $(\boldsymbol{y}_1, \boldsymbol{x}_1), \ldots, (\boldsymbol{y}_n, \boldsymbol{x}_n)$.
- Model assumption 1: Conditional distribution $F(\boldsymbol{y}_i | \boldsymbol{x}_i)$ given $\boldsymbol{x}_i$, $i = 1, \ldots, n$ is from pre-specified class of K-parametric densities

$$p(\boldsymbol{y}_i | \vartheta_{i1}, \ldots, \vartheta_{iK}).$$

- Model assumption 2: Each parameter ϑ_{ik}, $k = 1, \ldots, K$ is related to a regression predictor $\eta_{ik} = \eta_k(\boldsymbol{x}_i)$:

$$\vartheta_{ik} = h_k(\eta_{ik}) \text{ and } \eta_{ik} = h_k^{-1}(\vartheta_{ik})$$

However, . . .

establishing a good distributional model is difficult in practice because you need to decide

- which parametric distribution assumption to pick,
- which variable goes in which predictor (location, scale, shape of the distribution),

Our General Idea

- Extract the implicit copula of a response vector from a Bayesian regularized smoother
- Construct and compare copulas for:
  - Three popular shrinkage priors (BVS, PS, HS)
  - Differing (matching) bases

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  - Can be used to compare the shrinkage properties of any Bayesian smoother
  - Combined with arbitrary margins, the copula models provide a novel class of semiparametric distributional regression models

Sklar's Theorem

Consider N realizations $\boldsymbol{Y}_{(N)} = (Y_1, \ldots, Y_N)'$ of a continuous-valued response, with corresponding covariate values $\boldsymbol{x}_{(N)} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ Following Sklar's theorem the joint density of $\boldsymbol{Y}_{(N)}|\boldsymbol{x}_{(N)}$ can always be written as

$$p(\boldsymbol{y}_{(N)}|\boldsymbol{x}_{(N)}) = c^{\dagger}(F(y_1|\boldsymbol{x}_1), \ldots, F(y_N|\boldsymbol{x}_N)|\boldsymbol{x}) \prod_{i=1}^{N} p(y_i|\boldsymbol{x}_i)\,, \quad \text{for } N \geq 2$$

Here, $c^{\dagger}(\boldsymbol{u}_{(N)}|\boldsymbol{x}_{(N)})$ is a N-dimensional copula density and $F(y_i|\boldsymbol{x}_i)$ is the distribution function of $Y_i|\boldsymbol{x}_i$; both of which are unknown

Copula Smoother

- We model the joint density (given any covariates) using the copula decomposition

$$p(\boldsymbol{y}_{(N)}|\boldsymbol{x}_{(N)}) = c_\pi(F_Y(y_1), \ldots, F_Y(y_n)|\boldsymbol{x})\prod_{i=1}^{n} p_Y(y_i)$$

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- However, the impact of the covariate values on $\boldsymbol{Y}_{(N)}$ is captured through the copula with density $c_\pi(\boldsymbol{u}_{(N)}|\boldsymbol{x}_{(N)}, \boldsymbol{\theta})$, where $u_i = F_Y(y_i)$
- We call this a copula smoother because the relationship between $\boldsymbol{x}$ and $\boldsymbol{y}$ comes from the copula only

Construction of c_π

- c_π is constructed from a random vector $\tilde{\boldsymbol{Z}}$ with CDF $F_{\tilde{Z}}$ by inversion of Sklar's theorem:

$$C_\pi(\boldsymbol{u}|\boldsymbol{x}) = F_{\tilde{Z}}\left(F_{\tilde{Z}_1}^{-1}(u_1|\boldsymbol{x}), \ldots, F_{\tilde{Z}_n}^{-1}(u_n|\boldsymbol{x})|\boldsymbol{x}\right)$$

- $\tilde{Z}|\boldsymbol{x}$ is called pseudo response as it is not observed directly
- $u_1, \ldots, u_n$ is called the copula data

The Pseudo Response Model

- For $i = 1, \ldots, n$ consider the regression model

$$\tilde{Z}_i = \tilde{m}(x_i) + \varepsilon_i, \quad \varepsilon_i \overset{\text{iid}}{\sim} \mathrm{N}(0, \sigma^2),$$

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Copula Construction

- Let $S(\boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{\gamma}) = \text{diag}(s_1, \ldots, s_n)$ with

$$\text{Var}(\tilde{Z}_i | \boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{\gamma}) = \frac{\sigma^2}{s_i^2}$$

- Set

$$\boldsymbol{Z} = \sigma^{-1} S(\boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{\gamma}) \tilde{\boldsymbol{Z}}$$

- Then, the copula of $\boldsymbol{Z} | \boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{\gamma}$ is a Gaussian copula with correlation matrix

$$R(\boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{\gamma}) = S(\boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{\gamma})(I + BP_{\gamma}(\boldsymbol{\theta})^{-1} B') S(\boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{\gamma})$$

- Label the copula function $C(\boldsymbol{u} | \boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{\gamma})$

Copula Construction

- If $\pi(\boldsymbol{\theta}, \boldsymbol{\gamma})$ is any proper density, then the implicit copula is

$$C_\pi(\boldsymbol{u}|\boldsymbol{x}) = \int C(\boldsymbol{u}|\boldsymbol{x}, \boldsymbol{\theta}, \boldsymbol{\gamma})\pi(\boldsymbol{\theta}, \boldsymbol{\gamma})\mathrm{d}(\boldsymbol{\theta}, \boldsymbol{\gamma})$$

- It is easy to show that this is a proper copula
- For the regularization priors, $C_\pi(\boldsymbol{u}|\boldsymbol{x})$ turns out to be far (!) from a Gaussian copula

Three Implicit Copulas

- P-spline copula (PSC)
  - AR(2) prior
  - $\boldsymbol{\theta} = \{\tau^2, \psi_1, \psi_2\}$, $\boldsymbol{\gamma} = \emptyset$
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- Horseshoe copula (HSC)
  - $\beta_j \sim \mathrm{N}(0, \lambda_j^2)$, $\lambda_j \sim \mathrm{C}^+(0, \tau)$, $\tau \sim \mathrm{C}^+(0, 1)$
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  - Matched with Fourier basis or radial basis
- Bayesian variable selection copula (BVSC)
  - $\boldsymbol{\beta}_\gamma \sim \mathrm{N}(\mathbf{0}, c(B_\gamma' B_\gamma)^{-1})$, $\pi(\boldsymbol{\gamma}) = \mathrm{Beta}(p - p_\gamma + 1, p_\gamma + 1)$
  - $\boldsymbol{\theta} = \emptyset$, $\boldsymbol{\gamma} = \{\gamma_1, \ldots, \gamma_p\}$
  - Matched with regression splines or radial basis

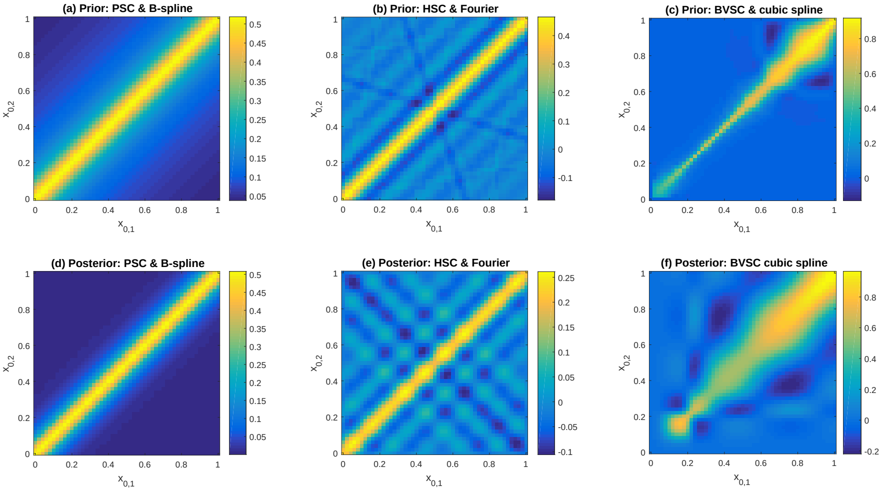
Dependence Structure

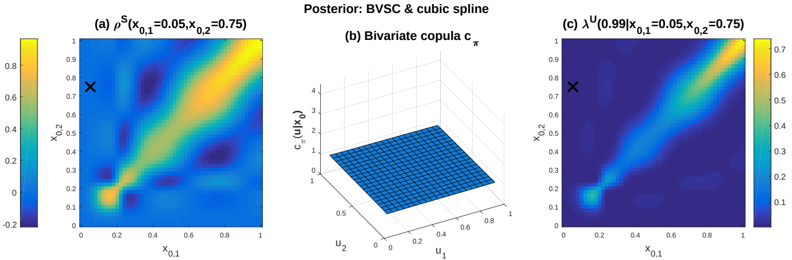
- For a univariate function $m(x)$ consider two new response values $Y_{0,1}, Y_{0,2}$ with covariate values $x_{0,1}, x_{0,2}$
- Compute the Spearman correlation

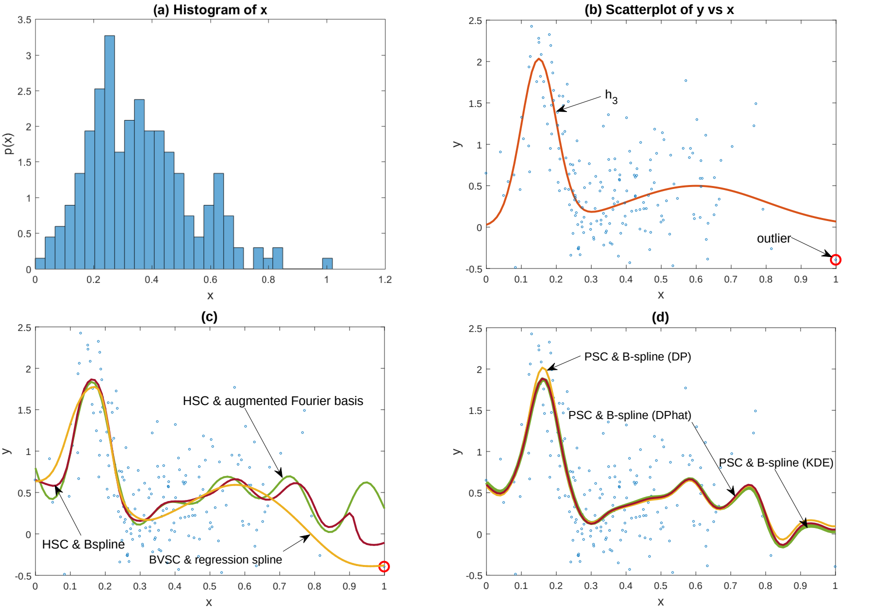
$$\rho_{\pi}^{S}(Y_{0,1}, Y_{0,2}|\boldsymbol{x}) \equiv \rho_{\pi}^{S}(Y_{0,1}, Y_{0,2}|\boldsymbol{x}, x_{0,1}, x_{0,2})$$

  and plot this as over a grid of $x_{0,1}, x_{0,2}$.
- We do this for $\pi(\boldsymbol{\theta}, \boldsymbol{\gamma})$ equal to the prior and the posterior

Dependence Structure




Posterior: BVSC & cubic spline
(a) ρ^S(x_{0,1}=0.05,x_{0,2}=0.75)
(b) Bivariate copula c_π
(c) λ^U(0.99|x_{0,1}=0.05,x_{0,2}=0.75)
x_{0,1}
x_{0,2}
c_π(u|x_0)
u_1
u_2



(a) Histogram of x
p(x)
x
(b) Scatterplot of y vs x
y
x
h3
outlier
(c)
y
x
HSC & augmented Fourier basis
HSC & Bspline
BVSC & regression spline
(d)
y
x
PSC & B-spline (DP)
PSC & B-spline (DPhat)
PSC & B-spline (KDE)

Posterior Estimation

- c_π cannot be expressed in closed form
- The conditional likelihood

$$p(\boldsymbol{y}|\boldsymbol{x}, \boldsymbol{\theta}, \gamma) = \phi_n(\boldsymbol{z}; \boldsymbol{0}, R(\boldsymbol{x}, \boldsymbol{\theta}, \gamma)) \prod_{i=1}^{n} \frac{p_Y(y_i)}{\phi_1(z_i)}$$

  is also computationally infeasible for large n because R is $(n \times n)$ and full
- Instead, we use the augmented likelihood

$$p(\boldsymbol{y}|\boldsymbol{x}, \beta, \boldsymbol{\theta}, \gamma)$$

  and MCMC
- Note that in contrast to the Bayesian linear model the posterior of $\boldsymbol{\theta}$ is often not available in closed form

Predictive Densities

- Predict the density of a new observation $Y_0|x_0$ using the posterior predictive density

$$p(y_0|x_0, \boldsymbol{x}, \boldsymbol{y}) = \int p(y_0|x_0, \boldsymbol{x}, \boldsymbol{\beta}, \boldsymbol{\theta}, \gamma) p(\boldsymbol{\beta}, \boldsymbol{\theta}, \gamma|\boldsymbol{x}, \boldsymbol{y}) \mathrm{d}(\boldsymbol{\beta}, \boldsymbol{\theta}, \gamma),$$

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- where

$$p(y_0|x_0,\boldsymbol{x},\beta,\boldsymbol{\theta},\gamma) = p(z_0|x_0,\boldsymbol{x},\beta,\boldsymbol{\theta},\gamma)\frac{p_Y(y_0)}{\phi_1(z_0)},$$

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  with $z_0 = \Phi^{-1}(F_Y(y_0))$
- Easy to compute MC estimates of density, and its moments (or other summaries) accurately

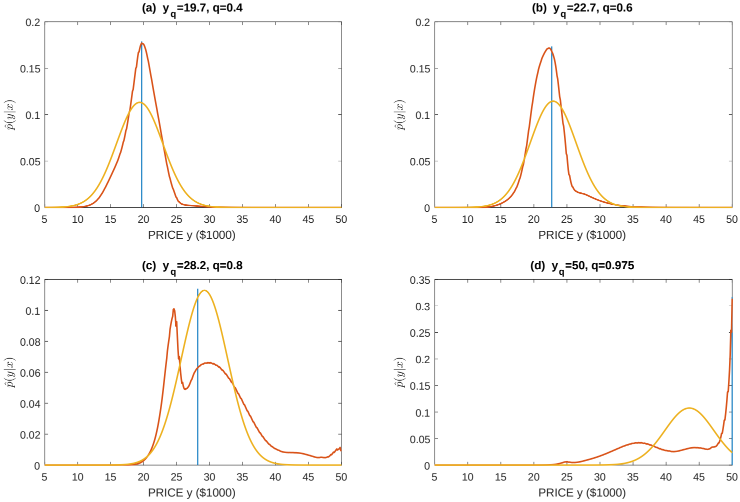
Motivating Example: Predicting House Prices

- Pseudo response model:

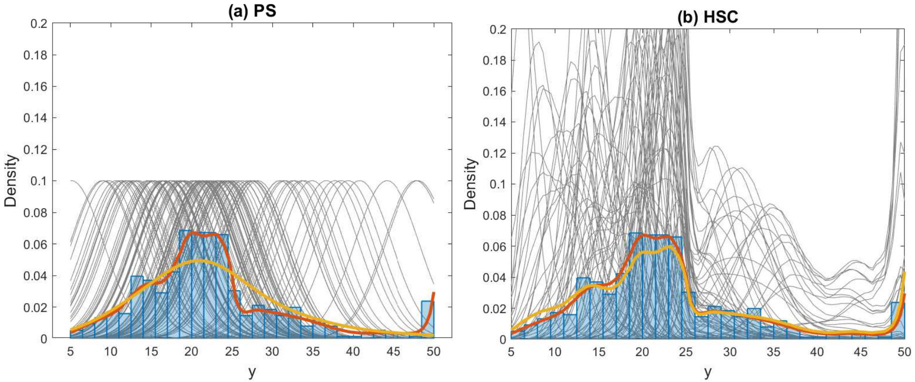
$$\tilde{Z}_i = \sum_{k=1}^{5} f(x_{ik}) + \varepsilon_i$$

- Major aim: Predictive densities of four house prices
- These are at 0.4,0.6,0.8,0.975 quantiles of the data distribution
- Comparison with a regular P-spline regression model (with Gaussian disturbances)
- Log-scores clearly favour the copula model
- We also compared results to other distributions (log-normal and Gamma) but results stayed similar.

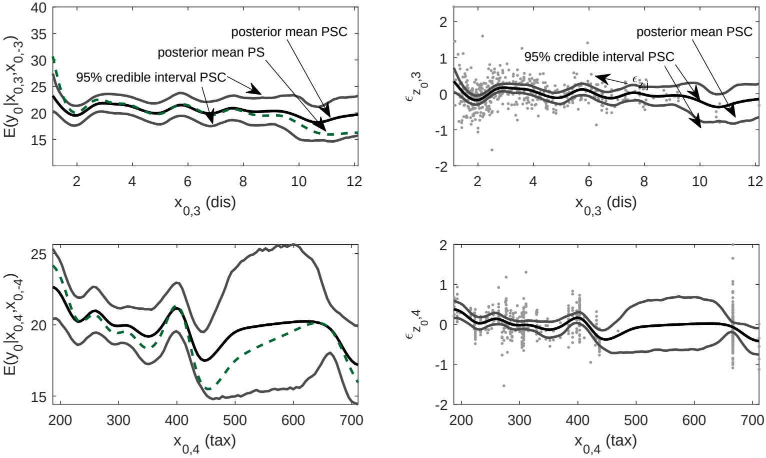
Predicting House Prices I



Predicting House Prices II



Predicted Expectations and Pseudo Residuals



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- New distributional regression method
- All dependence between Y and x is captured through a flexible implicit copula
- Improves predictive accuracy
- Applicable to multiple covariates and large n (e.g. 40,000 in other work)