Multivariate density estimation via copulas

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Outline

What is a copula?

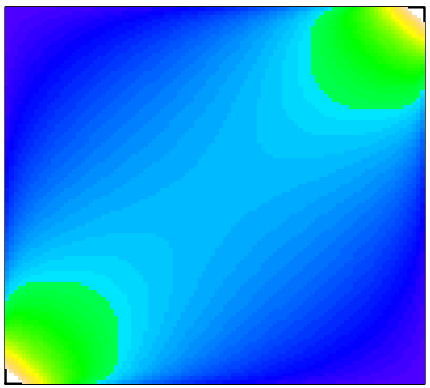
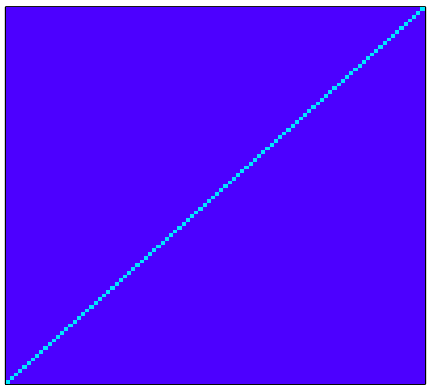
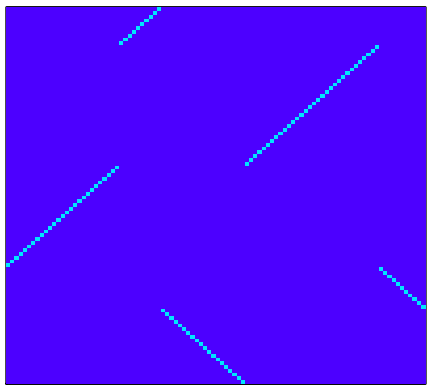
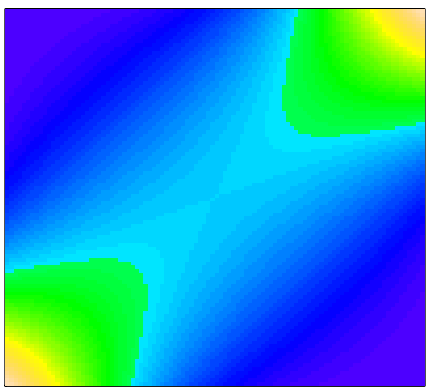
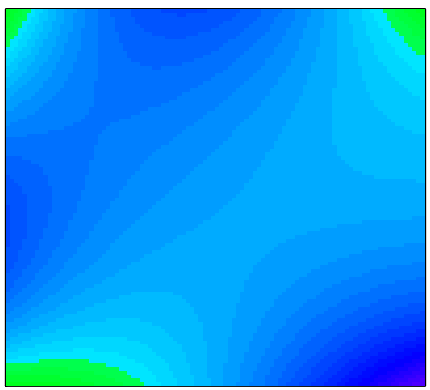
A *copula density* is a multivariate probability density on $[0,1]^2$ having uniform marginals:

$$p_1(u) = \int_0^1 p(u_1, u_2)\, du_2 = 1 \qquad p_2(u) = \int_0^1 p(u_1, u_2)\, du_1 = 1$$

More generally, a copula refers to the CDF of such a density:
$C : [0,1]^p \to [0,1]$ is a copula if

- C is increasing.
- $C(1, \ldots, 1, u_k, 1, \ldots, 1) = u_k$;
- $C(u_1, \ldots, u_p) = 0$ if $\min\{u_1, \ldots, u_p\} = 0$;

What do they look like?


Why use copulas?

Any multivariate distribution can be completely described by its copula and its univariate distributions:

Sklar's Theorem: Let F be a p-dimensional CDF and $F_1, \ldots, F_p$ the univariate margins. Then there exists a copula C such that

$$F(y_1, \ldots, y_p) = C(F_1(y_1), \ldots, F_p(y_p))$$

Think in terms of changes of variables. If F is continuous,

$$(y_1, \ldots, y_p) \sim F \leftrightarrow \left\{ \begin{array}{c} u_k = F_k(y_k) \\ y_k = F_k^{-1}(u_k) \end{array} \right\} \leftrightarrow (u_1, \ldots, u_p) \sim C$$

"Copulas are of interest for two main reasons (N. Fisher)":

1. a way of studying scale-free measures of dependence;
2. a starting point for constructing families of multivariate distributions.

they also allow us to divide multivariate density estimation into two parts:

univariate density estimation and copula estimation

Scale-free measures of dependence

"Kendall's τ": $(y_{i,1}, y_{i,2})$ and $(y_{j,1}, y_{j,2})$ are a concordant pair if $(y_{i,1} - y_{j,1}) \times (y_{i,2} - y_{j,2}) > 0$, otherwise they are discordant.

$$\hat{\tau} = \frac{1}{\binom{n}{2}}(c - d)$$

"Spearman's ρ": Let $r_{i,j}$ be the rank of $y_{i,j}$ among variable $\{y_{1,j}, \ldots, y_{n,j}\}$, $i = \{1, \ldots, n\}$, $j \in \{1, 2\}$.

$$\hat{\rho} = \mathrm{Cor}[(r_{1,1}, \ldots, r_{n,1}), (r_{1,2}, \ldots, r_{n,2})]$$

Both of these are invariant to monotone transformations of the variables, and thus depend on the copula and not the marginals. A variety of other dependence measures are derivable from the copula.

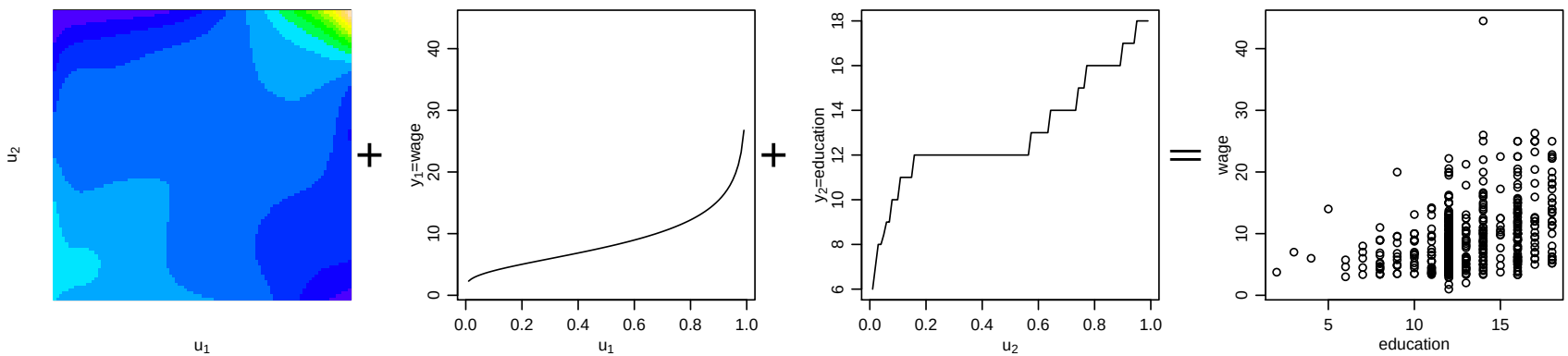
Latent variable model for multivariate distributions

Consider the following model: Let c be a copula density, and $G_1, \ldots, G_p$ be increasing functions with domain $[0, 1]$.

1. $\mathbf{u} = \{u_1, \ldots, u_p\} \sim c$ be latent variables.
2. $\mathbf{y} = \{y_1, \ldots, y_p\} = \{G_1(u_1), \ldots, G_p(u_p)\}$ be the observed data.

Then

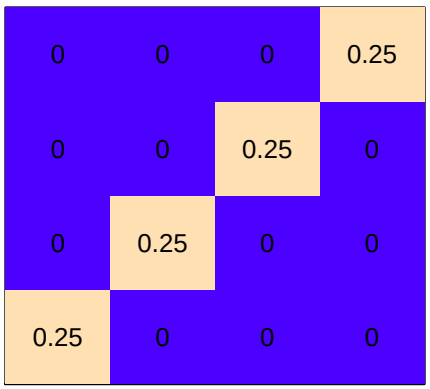
- c models the multivariate dependence,and
- $G_1 = F_1^{-1}, \ldots, G_p = F_p^{-1}$ model the univariate distributions.

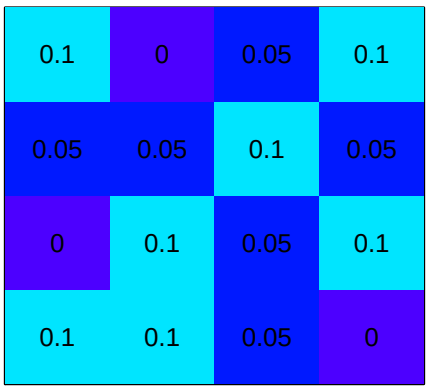


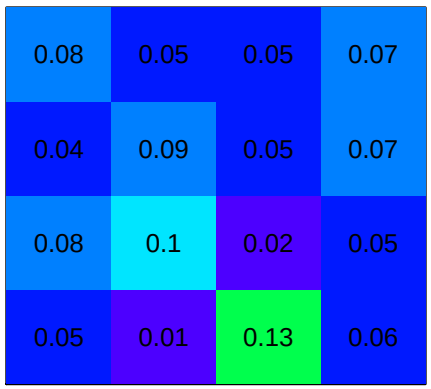
Discrete copulas

Doubly stochastic: A $K \times K$ matrix $\mathbf{M}$ is called doubly stochastic if it is positive and $\mathbf{M1} = \mathbf{M}^T\mathbf{1} = \mathbf{1}$.

Discrete copula: If $\mathbf{M}$ is doubly stochastic then $\mathbf{M}/K$ is a discrete copula, a distribution on $\{\frac{1}{K}, \frac{2}{K}, \ldots, \frac{K}{K}\}^2$ with uniform marginals.







Smoothed copulas

A discrete copula can be smoothed out: $\mathbf{f} = (f_1, \ldots, f_K)^T : [0,1] \to \mathbb{R}^K$ such that

(f1) each f_k is a probability density on $[0,1]$, and

(f2) $\sum_{k=1}^{K} f_k(u) = 1$ for all $u \in [0,1]$.

By straightforward integration it can be shown that the function

$$p(u_1, u_2 | K, \mathbf{M}) = \frac{1}{K} \mathbf{f}(u_1)^T \mathbf{M} \mathbf{f}(u_2)$$

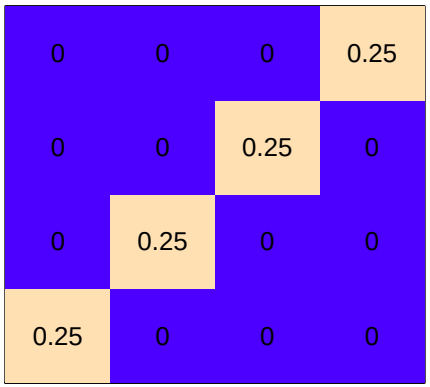
is a copula density on $[0,1]^2$ for any doubly stochastic matrix $\mathbf{M}$.

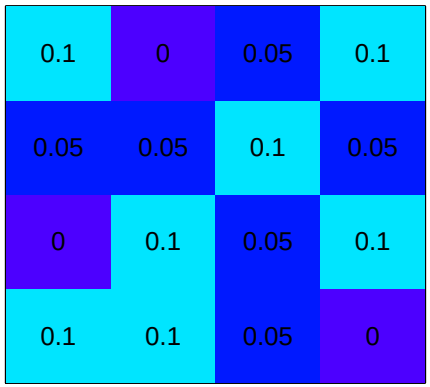
One such $\mathbf{f}$ is the set of beta densities with integer (a, b), $a + b = K + 1$:

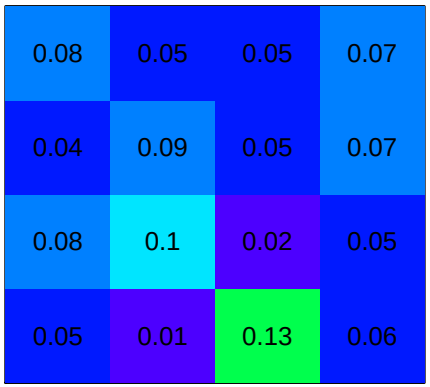
$$\mathbf{f}(u) = \{\texttt{dbeta(u, 1, K)}, \texttt{dbeta(u, 2, K} - 1\texttt{)}, \ldots, \texttt{dbeta(u, K, 1)}\}$$

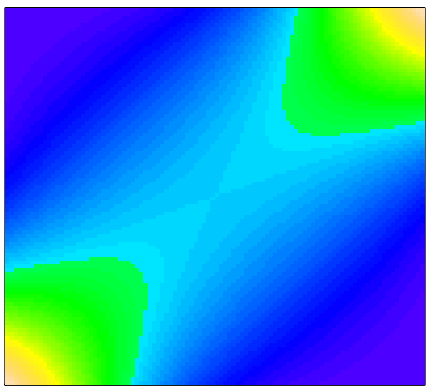
Such an $\mathbf{f}$ is essentially a Bernstein polynomial, and the resulting copula is called a Bernstein copula.

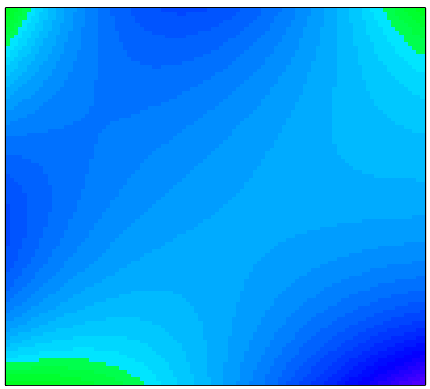
How things get smoothed











Multivariate extension

Another way to write out the model is

$$p(u_1, u_2|\mathbf{M}) = \sum_{k_1=1}^{K} \sum_{k_2=1}^{K} \mathbf{M}_{k_1,k_2} f_{k_1}(u_1) f_{k_2}(u_2)$$

This extends to higher dimensional densities as

$$p(\mathbf{u}|\mathbf{M}) = \sum_{k_1=1}^{K} \cdots \sum_{k_p=1}^{K} \mathbf{M}_{k_1,\ldots,k_p} \prod_{j=1}^{p} f_{k_j}(u_j)$$

This can be seen as a latent class model:

1. Sample a latent class vector $\mathbf{k} \in \{1, \ldots, K\}^p$ according to $\mathbf{M}$;
2. Sample $\mathbf{u}|\mathbf{k} \sim \prod_{j=1}^{p} f_{k_j}(u_j)$.

Then $\mathbf{u}$ is a sample from $p(\mathbf{u}|\mathbf{M})$.

Estimation I

- Sancetta and Satchell (2004):
  1. Pick K as a function of n, based on an asymptotic result;
  2. Let $\hat{\mathbf{M}}$ be the empirical proportions in the $K \times K$ bins;
  3. Let $\hat{p}(u_1, u_2) = \frac{1}{K}\mathbf{f}(u_1)^T \hat{\mathbf{M}} \mathbf{f}(u_2)$.
     Warning: not actually a copula density!
- Maximum likelihood:
  1. The parameter space for $\mathbf{M}$ is a compact convex set.
  2. Use Newton's method with a logarithmic barrier to minimize $-\sum_{i=1}^{n} \log p(u_{i,1}, u_{i,2}|\mathbf{M})$.
  3. Compare values of K using AIC, BIC or something similar.

Question: Wait a minute, are $(u_{1,1}, u_{1,2}), \ldots, (u_{n,1}, u_{n,2})$ actually observed?

Answer: No. People generally plug-in $\hat{u}_{i,j} = \hat{F}(y_{i,j})$.

Research goals

Problems with the aforementioned approaches:

- The $u_{i,j}$'s not actually observed - uncertainty in their value is not accounted for (this is primarily a concern if the $y_{i,j}$'s are discrete).
- In S&S's approach the estimate isn't actually a copula.
- In the MLE approach things get pretty messy in higher dimensions.
- In some cases we may want the coarseness of $\mathbf{M}$ to be different across the p variables.

Maybe we can solve these problems and/or make everything more complicated. I propose to do this by constructing a mixture model for copula densities that mix over simple Bernstein copulas of varying coarseness.

Choquet's theorem

Bivariate Bernstein copula: $\mathbf{M} \in \mathcal{M}_K = \{\text{stochastic } K \times K \text{ matrices}\}$.

Choquet's theorem: $\mathcal{M}_K$ is a compact, convex set. Every $\mathbf{M} \in \mathcal{M}_K$ can therefore be expressed as a mixture over the extreme points (vertices) of $\mathcal{M}_K$.

$$\mathbf{M} \in \mathcal{M}_K \Leftrightarrow \mathbf{M} = \sum w(\mathbf{S})\mathbf{S}$$

In other words, the

constrained estimation problem (estimation of $\mathbf{M} \in \mathcal{M}_K$)

can be re-expressed as an

unconstrained mixture estimation problem (estimation of $w(\mathbf{S})$).

Permutation matrices

The extreme points of $\mathcal{M}_K$ are the
permutation matrices: stochastic matrices consisting of zeros and ones.

$$\mathbf{S}_1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad \mathbf{S}_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \mathbf{S}_3 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

Note that these can be expressed as $K \times 2$ matrices

$$\mathbf{A}_1 = \begin{pmatrix} 1 & 1 \\ 2 & 2 \\ 3 & 3 \\ 4 & 4 \end{pmatrix} \quad \mathbf{A}_2 = \begin{pmatrix} 1 & 4 \\ 2 & 3 \\ 3 & 1 \\ 4 & 2 \end{pmatrix} \quad \mathbf{A}_3 = \begin{pmatrix} 1 & 1 \\ 2 & 3 \\ 3 & 4 \\ 4 & 2 \end{pmatrix}$$

Extreme Bernstein density:

$$p(u_1, u_2|\mathbf{S}) = \frac{1}{K} \sum_{k_1=1}^{K} \sum_{k_2=1}^{K} \mathbf{S}_{k_1,k_2} f_{k_1}(u_1) f_{k_2}(u_2) = \frac{1}{K} \sum_{k=1}^{K} f_{\mathbf{A}_{k,1}}(u_1) f_{\mathbf{A}_{k,2}}(u_2)$$

Permutation arrays

This idea can be extended beyond two dimensions:

Stochastic arrays: Let $\mathcal{M}_K$ be the set of K^p-dimensional stochastic arrays

Extreme points: Stochastic arrays consisting of ones and zeros $\Rightarrow$ multivariate permutation arrays.

$$\begin{pmatrix} 1 & 1 & 4 \\ 2 & 2 & 3 \\ 3 & 3 & 2 \\ 4 & 4 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 4 & 1 \\ 2 & 3 & 2 \\ 3 & 1 & 4 \\ 4 & 2 & 3 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 & 2 \\ 2 & 3 & 1 \\ 3 & 4 & 3 \\ 4 & 2 & 4 \end{pmatrix}$$

Extreme Bernstein density: $p(\mathbf{u}|\mathbf{A}) = \frac{1}{K} \sum_{k=1}^{K} \left\{ \prod_{j=1}^{p} f_{\mathbf{A}_{k,j}}(u_j) \right\}$

Rectangular permutation arrays

Suppose u_1 and u_2 are highly dependent, but independent of u_3. It will take a mixture of many extreme Bernstein copulas to represent this.

To obtain a more efficient representation, consider permutation arrays of the form

$$\begin{pmatrix} 1 & 1 & 1 \\ 2 & 2 & 1 \\ 3 & 3 & 1 \\ 4 & 4 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 1 & 1 \\ 2 & 1 & 1 \\ 3 & 2 & 1 \\ 4 & 2 & 1 \end{pmatrix} \quad \begin{pmatrix} 1 & 4 & 1 \\ 2 & 2 & 2 \\ 3 & 3 & 2 \\ 4 & 1 & 1 \end{pmatrix}$$

Each column of $\mathbf{A}$ is a permutation of K/K_j copies of $\{1, \ldots, K_j\}$. We have restricted K/K_j to be a power of 2. The density $p(\mathbf{u}|\mathbf{A}) = \frac{1}{K} \sum_{k=1}^{K} \left\{ \prod_{j=1}^{p} f_{\mathbf{A}_{k,j}}(u_j) \right\}$ is still a copula density.

Mixtures of Bernstein copulas

Mixture model: Any copula density can be approximated by a mixture of the form

$$p(\mathbf{u}|q) = \int_{\mathbf{A}} p(\mathbf{u}|\mathbf{A}) q(d\mathbf{A}).$$

The mixing measure q is unknown and to be estimated. It is a measure over rectangular permutation arrays of various shapes and sizes.

Estimation II

We generally don't observe data $\mathbf{u}_1, \ldots, \mathbf{u}_n$ with uniform marginals. What does the observed data tell us about $\mathbf{u}_1 \ldots, \mathbf{u}_n$?

$$D = \{\mathbf{u}_1, \ldots, \mathbf{u}_n : u_{i_1,j} < u_{i_2,j} \text{ if } y_{i_1,j} < y_{i_2,j}\}$$

The "partial likelihood" is

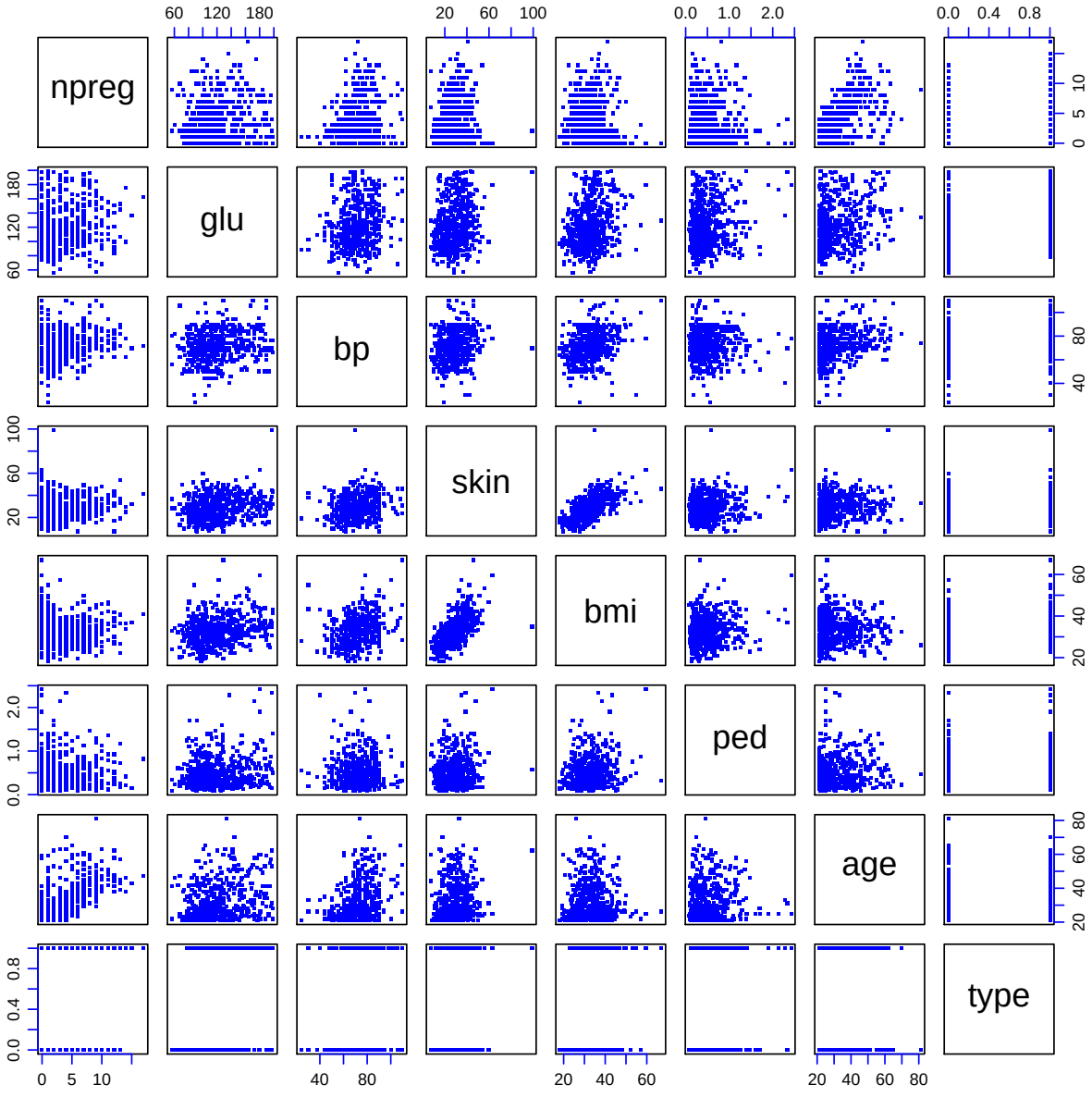
$$p(D|q) = \int_D \left\{ \prod_{i=1}^{n} p(\mathbf{u}_i|q) d\mathbf{u}_i \right\}$$

We will consider penalbayesized estimates which achieve high values of the following objective function

$$f(q|\mathbf{u}_1, \ldots, \mathbf{u}_n) = \log p(D|q) + \log \pi(q)$$

As you might guess, there are MCMC schemes to obtain such estimates.

Diabetes data



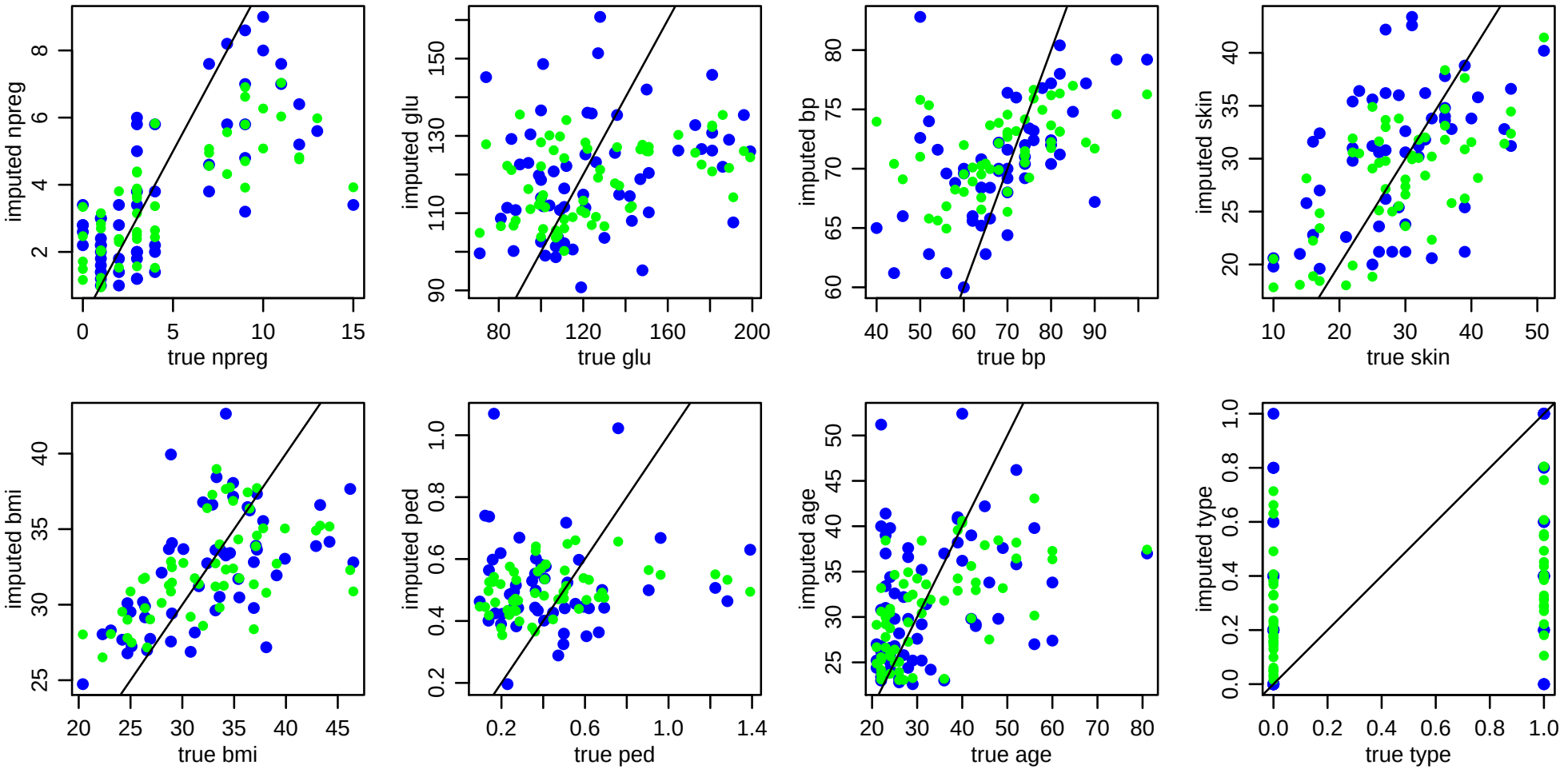
Imputation experiment

Experiment: Given data on $p = 8$ variables for $n = 532$ women,

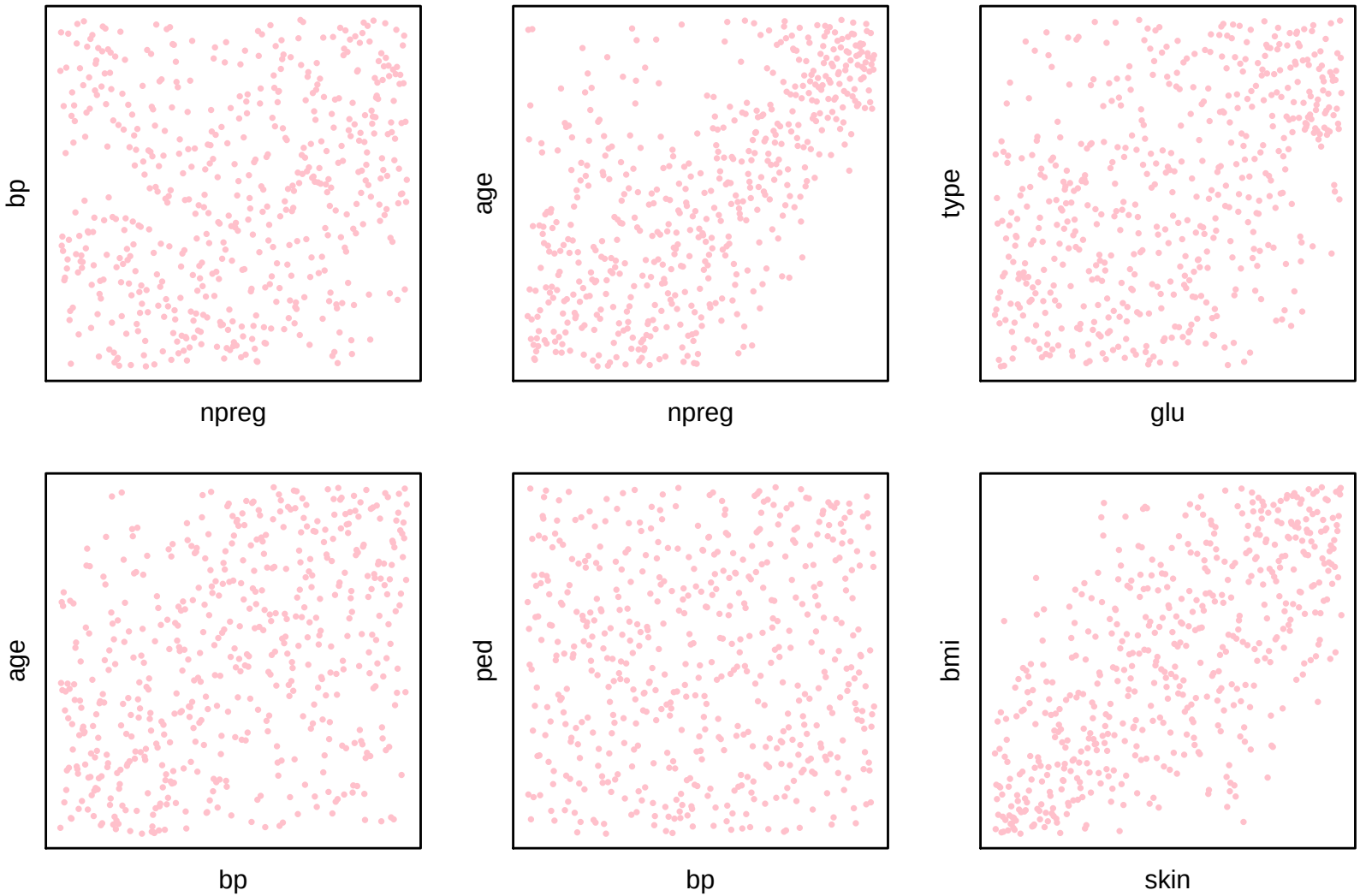
1. replace 10% of data with missing values;
2. obtain posterior mean $\hat{y}^b_{i,j}$ of $y_{i,j}$ for each missing value;
3. obtain 5-nearest-neighbor estimate $\hat{y}^n_{i,j}$ of $y_{i,j}$ for each missing value;
4. compare $\hat{\mathbf{y}}^b$ and $\hat{\mathbf{y}}^n$ to actual values.

variable	Bayes error$_B^{1/2}$	Bayes error$_G^{1/2}$	KNN error$^{1/2}$	MSE$^{1/2}$
npreg	0.92	0.95	0.90	1.25
glu	1.01	0.99	1.07	1.08
bp	0.97	0.97	0.90	1.07
skin	0.66	0.67	0.82	0.88
bmi	0.73	0.74	0.74	0.88
ped	0.82	0.82	0.96	0.86
age	0.96	0.98	1.15	1.16
type	0.97	0.93	0.99	1.04

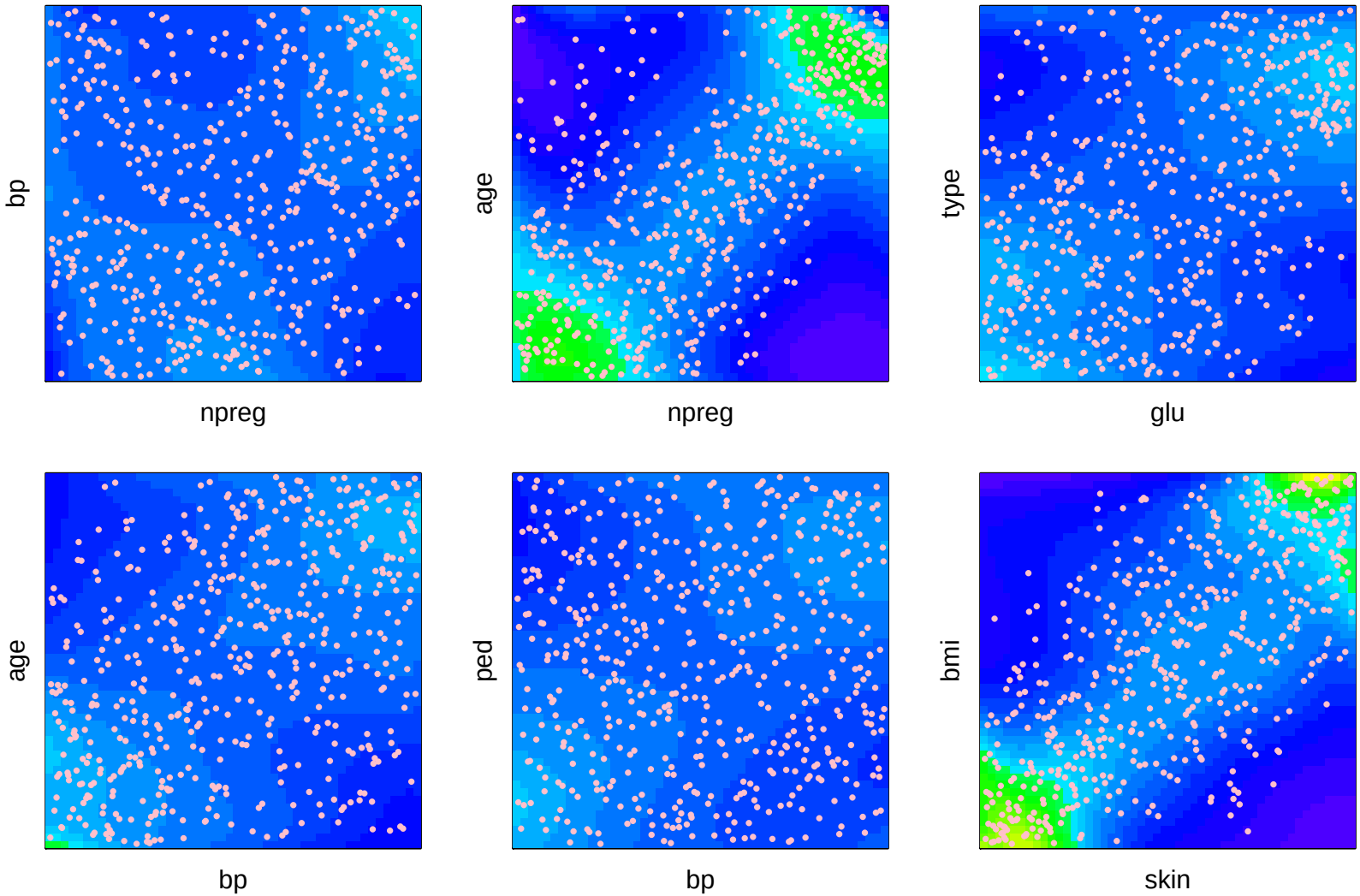
Imputation experiment



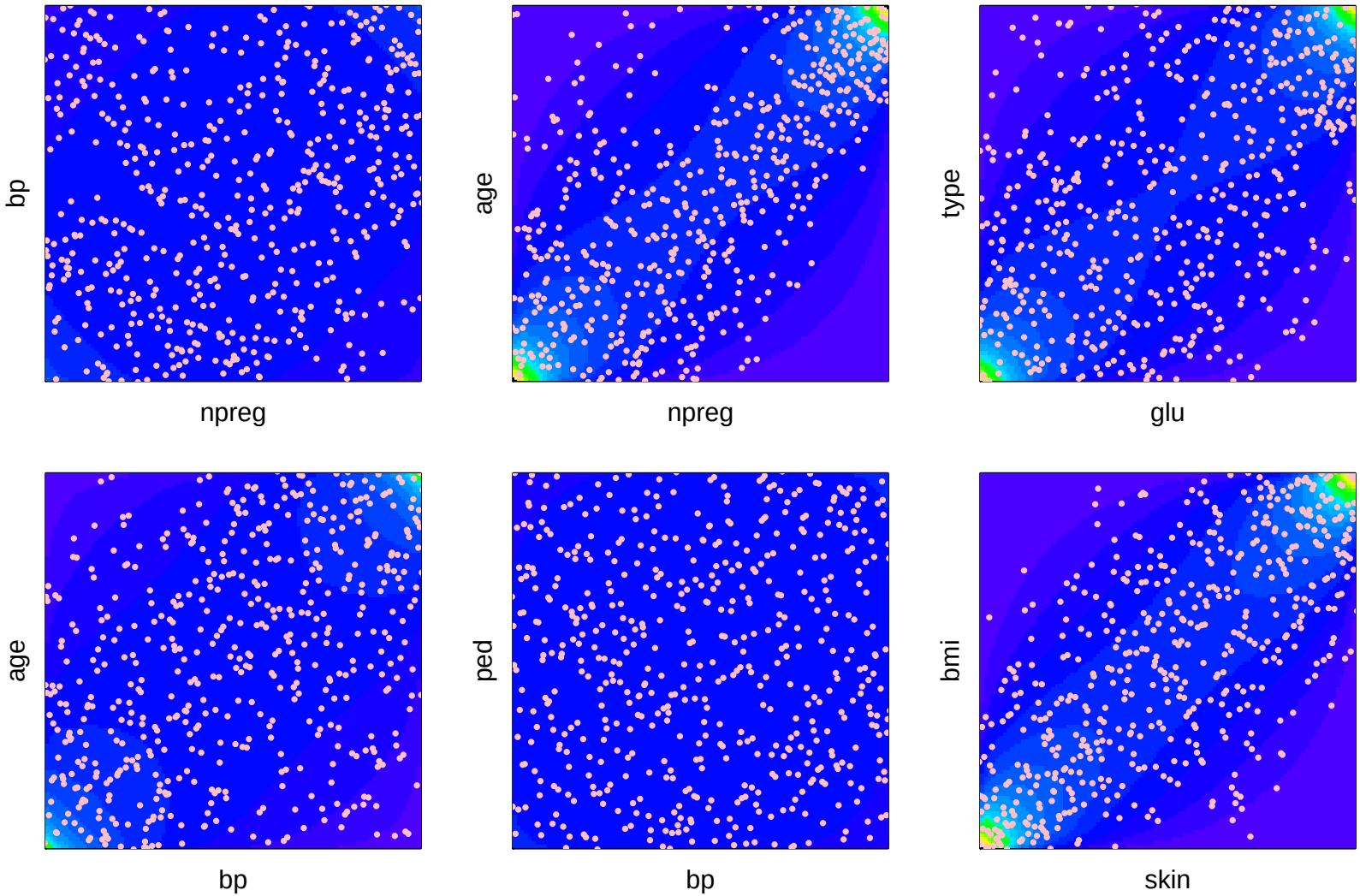
Estimates of bivariate marginals: Raw data



Estimates of bivariate marginals: Bernstein copula



Estimates of bivariate marginals: Gaussian copula



Summary

Future work