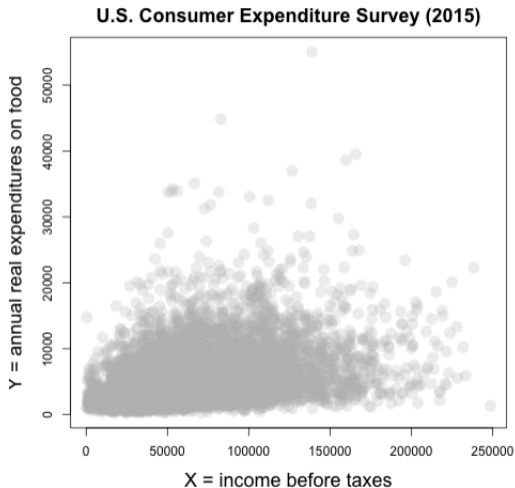


# On super-level sets of conditional multivariate densities for multiple-output quantile regression \*

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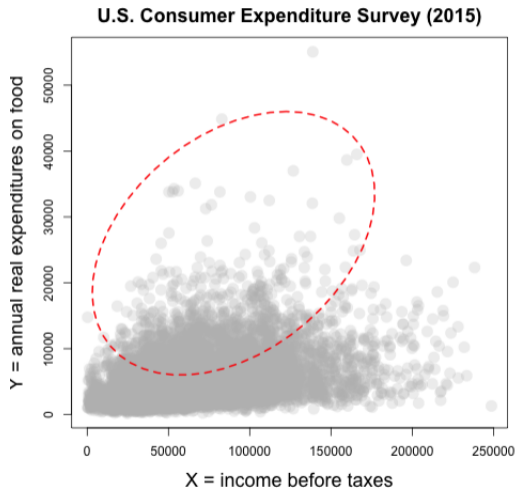
\* Joint work with Annika Camehl and Dennis Fok

# Example: Heterogeneity in Household Consumption Patterns



►  $\{y_n, x_n\}_{n=1}^N$  and  $N = 29,988$

# Example: Heterogeneity in Household Consumption Patterns

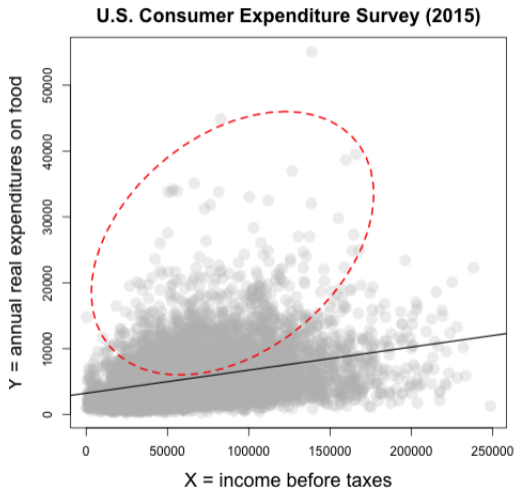


▶  $\{y_n, x_n\}_{n=1}^N$  and  $N = 29,988$

▶  $y_n = \mu + x_n' \beta + u_n$

Assume, our interest is in the “top”  
(i.e., 10%) household segment.

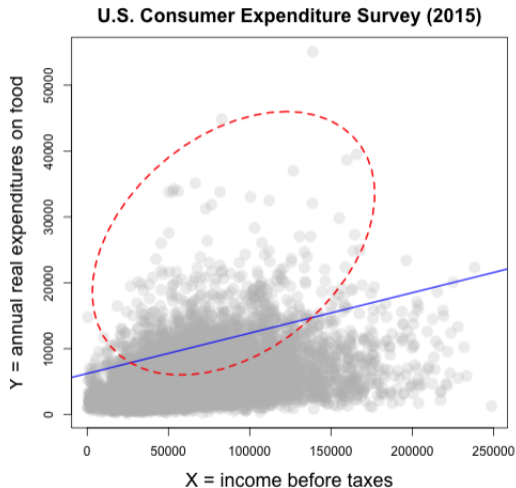
# Example: Heterogeneity in Household Consumption Patterns



Mean regression

$$\bar{m}(x_n) = \mu + x'_n \beta$$

# Example: Heterogeneity in Household Consumption Patterns

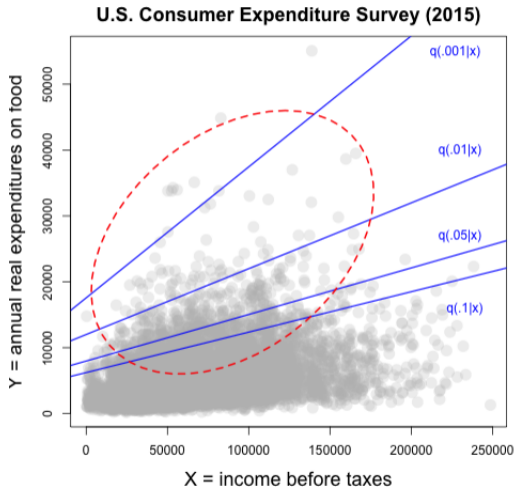


Quantile regression

$$q(.1|x_n) = \mu_{(.1)} + x_n' \beta_{(.1)}$$

Provides insights into the effects of covariates that are missed with mean regression!

# Example: Heterogeneity in Household Consumption Patterns



Quantile regression

$$\left\{ q(\alpha_l | x_n) = \mu(\alpha_l) + x_n' \beta(\alpha_l) \right\}_{l=1}^L$$

Provides a comprehensive picture of the conditional response distribution!

## **Study of heterogeneity in treatment participation**

(e.g., Abadie, Angrist & Imbens, 2002; Athey & Imbens 2006; Firpo, 2007; Chernozhukov & Hansen, 2013)

## **Value-at-risk (tail value) measurement**

(Chernozukov & Umantsev, 2001; Engle & Manganelli, 2004)

## **Exploration of multiple-output and functional responses**

(Hallin, Paindaveine & Siman, 2010; Wei 2008; Carlier, Chernozhukov & Galichon, 2016, Hallin & Siman, 2016; **this talk!**)

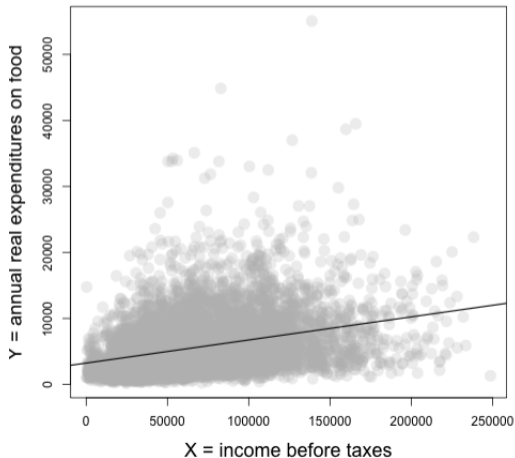
# This Talk

- ▶ The quantile is defined as a property of an (estimated) conditional multivariate density.
- ▶ This so-called super-level set enables a clear probabilistic interpretation and enjoys favorable quantile properties.
- ▶ Linear and non-linear multivariate as well as univariate regression quantiles are obtained in a comprehensive (fully) Bayesian framework.



# Regression Quantiles in a Nutshell

(Conditional) mean regression

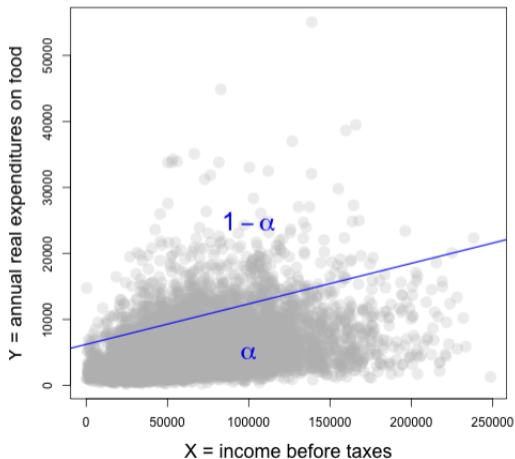


$$\operatorname{argmin}_{\mu, \beta} \sum_{n=1}^N |y_n - \bar{m}(x_n)|^2$$

⇒ solved with numerical linear algebra (i.e., OLS).

# Regression Quantiles in a Nutshell

(Conditional) quantile regression



$$\operatorname{argmin}_{\mu(\alpha), \beta(\alpha)} \sum_{n=1}^N \rho_{\alpha} |y_n - q(\alpha | x_n)|$$

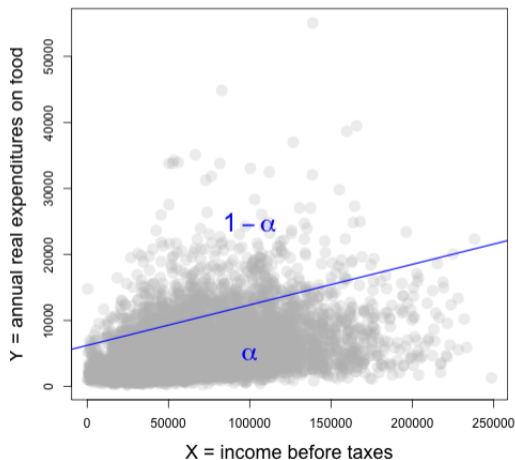
for  $0 < \alpha < 1$ , and asymmetric weight (“check”) function:

$$\rho_{\alpha}(u_n) = \begin{cases} \alpha u_n, & u_n > 0 \\ -(1 - \alpha) u_n, & u_n \leq 0 \end{cases}$$

$\Rightarrow$  solved with linear programming  
(see, Koenker & Bassett, 1978).

# Regression Quantiles in a Nutshell

(Conditional) quantile regression



$$\rho_{\alpha}(u_n) = u_n(\alpha I_{(u_n > 0)} - (1 - \alpha) I_{(u_n \leq 0)})$$

equivalent to:

$$u_n \stackrel{iid}{\sim} \mathcal{AL}(0, \sigma, \alpha)$$

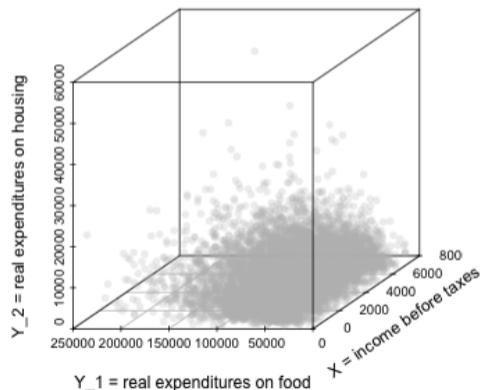
with asymmetry parameter  $0 < \alpha < 1$

Example

$\Rightarrow$  ML (and Bayesian) inference is straightforward (see, Koenker & Machado, 1999; Yu & Moyeed, 2001).

# Regression Quantiles in a Nutshell

Multiple-outputs:  $\mathbf{y}_n = (y_{n1}, \dots, y_{nK})'$



$$q(\alpha | \mathbf{x}_n) = \boldsymbol{\mu}_{(\alpha)} + \mathbf{B}_{(\alpha)} \mathbf{x}_n$$

where  $\boldsymbol{\mu}_{(\alpha)}$  is  $K \times 1$  and  $\mathbf{B}_{(\alpha)}$  is  $K \times G$

$\Rightarrow$  Seemingly unrelated regression, simultaneous equations, VAR ...

The conditional Koenker-Bassett quantile concept is not easy to extend!

## Attempt 1: Conditioning

$$\mathbf{q}(\alpha) = [q_{y_{n1}}(\alpha | \mathbf{y}_{n(-1)}), \dots, q_{y_{nK}}(\alpha | \mathbf{y}_{n(-K)})]'$$

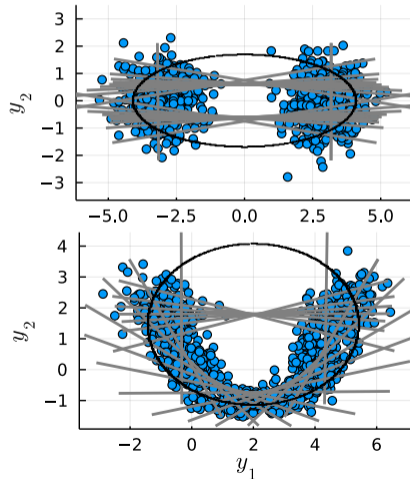
- ▶ Input-space augmentation, assumes all “regressors” are fixed!

# Multivariate Quantiles

## Attempt 2: Directional

- Convex intersection of  $\alpha$ -quantile halfspaces for different (Koenker-Bassett) regression hyperplanes (Hallin, Paindaveine & Siman, 2010).

Areas within the gray lines (contours) give the 80%-**directional** quantile (20 directions).



# Multivariate Quantiles

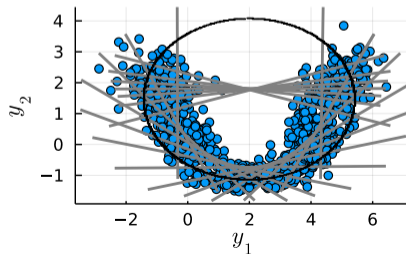
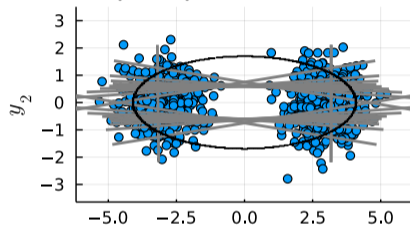
## Attempt 2: Directional

- ▶ Convex intersection of  $\alpha$ -quantile halfspaces for different (Koenker-Bassett) regression hyperplanes (Hallin, Paindaveine & Siman, 2010).

## Attempt 3: Direct

- ▶ Find an ellipsoid around a (determined) center with  $\alpha$ -probability mass (e.g., Hallin & Siman, 2016).

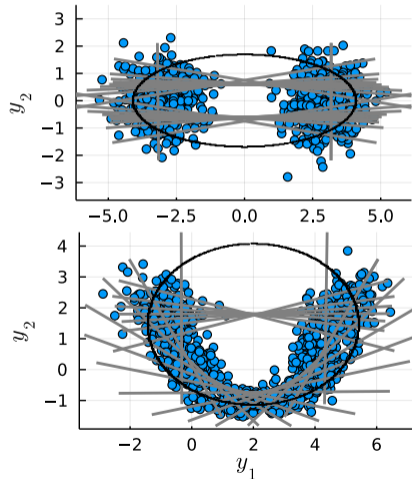
Areas within the black lines (countours) give the 80%-elliptical quantile.



# Multivariate Quantiles

- ▶ The (directional) quantile contours are not guaranteed to cover  $\alpha$ .
- ▶ The quantile regions can cover large parts with little to no probability mass.
- ▶ The definitions cannot easily be extended (i.e., to more than two outputs/ inputs).

Interpretability and practical use?





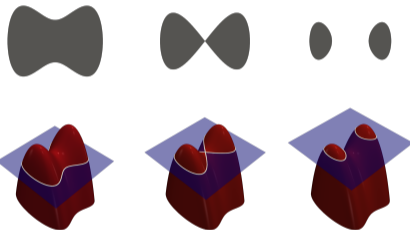
# Multivariate Quantiles

## Level set

$$\mathcal{L}(f; t) = \{ \mathbf{y}_n \in \mathbb{R}^K : f(\mathbf{y}_n) = t \}$$

$\Rightarrow$  Cross-section of  $f(\cdot)$  at a given (constant) value  $t$  (Osher & Sethian, 1988).

Level sets of a bivariate bimodal distribution for three different values of  $t$ .



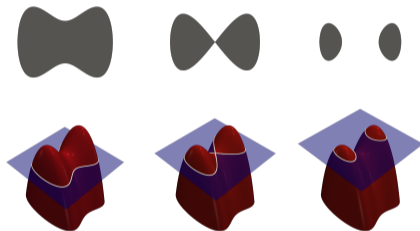
# Multivariate Quantiles

## Super-level set

$$\mathcal{L}(f; t) = \{ \mathbf{y}_n \in \mathbb{R}^K : f(\mathbf{y}_n) \geq t \}$$

for threshold  $t > 0$ , gives the highest density region for  $f(\cdot)$  (see, e.g., Hartigan, 1987).

Level sets of a bivariate bimodal distribution for three different values of  $t$ .



# Multivariate Quantiles

## Super-level set

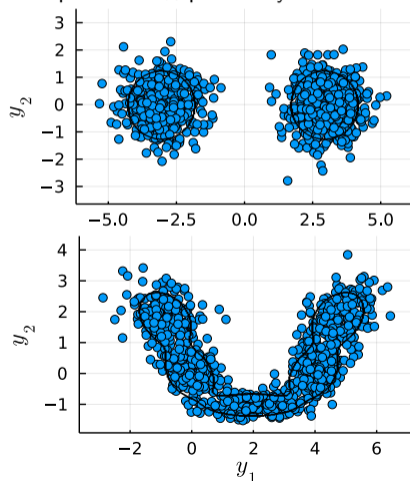
$$\mathcal{L}(f; t) = \{ \mathbf{y}_n \in \mathbb{R}^K : f(\mathbf{y}_n) \geq t \}$$

for threshold  $t > 0$ , gives the highest density region for  $f(\cdot)$  (see, e.g., Hartigan, 1987).

## Super-level set quantile

$$\mathbf{q}(\alpha) = \mathcal{L}(f; t_\alpha^*),$$
$$t_\alpha^* = \sup \{ Pr(\mathbf{y}_n \in \mathcal{L}(f; t)) \geq \alpha \}$$

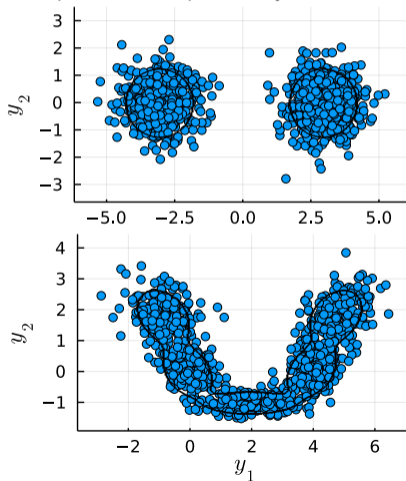
Areas within the lines (quantile contours) correspond to 80% probability mass.



# Multivariate Quantiles

- ▶ Supports a clear probabilistic interpretation (in terms of  $\alpha$ ).
- ▶ (Flexible) quantile regions cover areas with high probability mass.
- ▶ Extensions to more than two inputs/outputs are straightforward.

Areas within the lines (quantile contours) correspond to 80% probability mass.



# Properties

	Univariate quantile collection	Directional quantile	Elliptical quantile	Reference quantile (Wei, 2008)	Super-level set quantile
Vector-valued	no	✓	✓	✓	✓
$\alpha$ -probability coverage control	no	no	✓	✓	✓
Reflects probability mass concentration	no	no	no	no	✓
Nestedness	no	✓	✓	✓	✓
Uniqueness	✓	✓	✓	✓	✓
Affine equivariance	no	✓	✓	✓	✓
Invariant to coordinate transformations	✓	no	no	no	no
Invariant to monotone transformations	no	no	no	no	no
Reduces to classic univariate quantile	✓	no	no	no	no

# HPD vs. Super-Level Set Quantiles

## Highest posterior density set

- ▶ Operationalizes uncertainty of a model parameter for a (typically) univariate and unimodal posterior distribution (i.e., an interval, Box & Tiao, 1965).

## Super-level set

- ▶ Quantifies uncertainty in a (set of) response variable(s), conditional on other response variables, for arbitrarily shaped joint posterior distributions (i.e., an interval or a set of intervals).

# Let's go (fully) Bayesian

(Overfitted) Finite Gaussian Mixture Model:

$$f(\mathbf{y}_n | \mathbf{x}_n) = \sum_{m=1}^M \kappa_m \phi(\mathbf{g}_m(\mathbf{x}_n), \Sigma_m),$$

$$\text{where } \mathbf{g}_m(\mathbf{x}_n) = \boldsymbol{\mu}_m + \mathbf{B}_m \mathbf{x}_n,$$

$$\boldsymbol{\kappa} | \{\bar{\rho}_m\} \sim \mathcal{D}(\bar{\rho}_1, \dots, \bar{\rho}_M),$$

$$\bar{\rho}_m \sim \mathcal{G}(\underline{a}_1, 1/(\underline{a}_2 M)).$$

with  $M$  comparatively large (Nobile & Fearnside, 2007; Rousseau & Mengersen, 2011) and a **Shrinkage Prior** on  $\phi(\mathbf{g}_m(\mathbf{x}_n), \Sigma_m)$  (Malsiner-Walli, Frühwirth-Schnatter & Grün, 2016).

# Implementation

$$\boldsymbol{\mu}_m^{\mathcal{K}|\mathcal{C}}(\mathbf{y}_C, \mathbf{x}) = \mathbf{g}_{m,\mathcal{K}}(\mathbf{x}) + \boldsymbol{\Sigma}_{m,\mathcal{K},\mathcal{C}} \boldsymbol{\Sigma}_{m,\mathcal{C},\mathcal{C}}^{-1} (\mathbf{y}_C - \mathbf{g}_{m,\mathcal{C}}(\mathbf{x})),$$

$$\boldsymbol{\Sigma}_m^{\mathcal{K}|\mathcal{C}} = \boldsymbol{\Sigma}_{m,\mathcal{K},\mathcal{K}} - \boldsymbol{\Sigma}_{m,\mathcal{K},\mathcal{C}} \boldsymbol{\Sigma}_{m,\mathcal{C},\mathcal{C}}^{-1} \boldsymbol{\Sigma}_{m,\mathcal{C},\mathcal{K}},$$

$$\omega_m^{\mathcal{C}}(\mathbf{y}_C, \mathbf{x}) = \frac{\kappa_m \phi(\mathbf{g}_{m,\mathcal{C}}(\mathbf{x}), \boldsymbol{\Sigma}_{m,\mathcal{C},\mathcal{C}})}{\sum_{l=1}^M \kappa_l \phi(\mathbf{g}_{l,\mathcal{C}}(\mathbf{x}), \boldsymbol{\Sigma}_{l,\mathcal{C},\mathcal{C}})},$$

... serve as inputs to the Level-set algorithm to compute  $\tilde{\mathbf{q}}(\alpha)$ .



# Simulation Exercise

- 1 Multivariate Gaussian
- 2 Multivariate Student-t
- 3 Multivariate log-Gaussian
- 4 Conditional heteroskedasticity
- 5 Multivariate Gaussian mixture

1,000 data sets with a sample size of 10,000 for each `DGP`.

## Hyperparameters

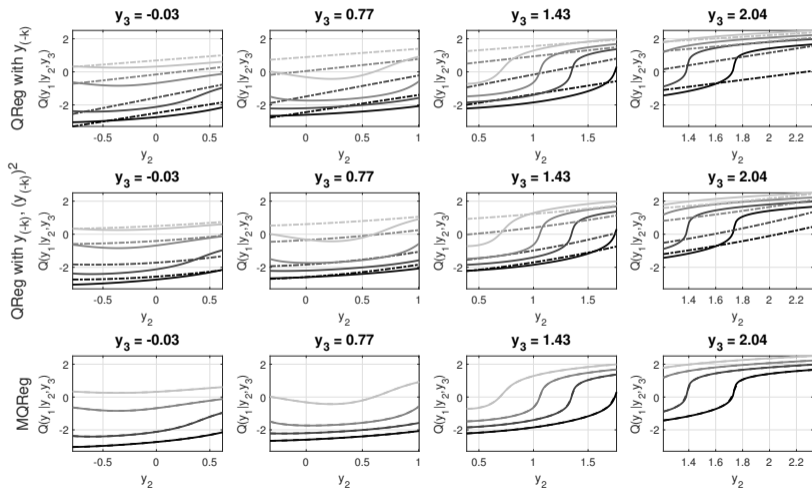
- ▶  $M = 5$
- ▶  $\underline{a}_1 = 10, \underline{a}_2 = 40$  (Dirichlet prior)
- ▶  $\underline{b}_1 = .5, \underline{b}_2 = .5$  (Gamma prior)

## MCMC samples

- ▶ Effective: 50,000 / 10  
(Burn-in: 10,000)

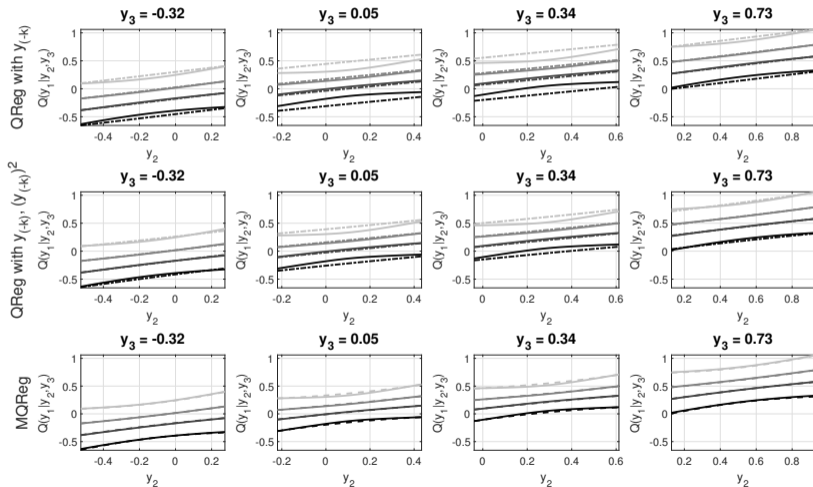
# Simulation Exercise: Multivariate Gaussian Mixture

Estimated (dashed lines) vs. true (solid lines) conditional quantiles for  $\alpha \in \{.2, .4, .6, .8\}$

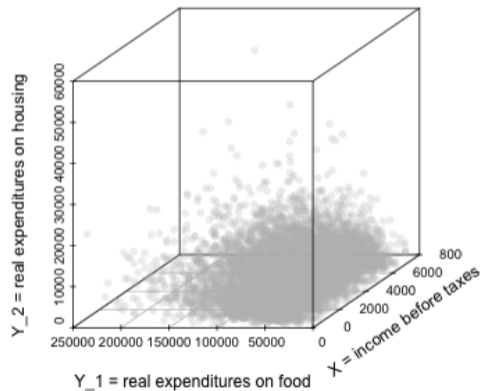


# Simulation Exercise: Conditional Heteroskedasticity

Estimated (dashed lines) vs. true (solid lines) conditional quantiles for  $\alpha \in \{.2, .4, .6, .8\}$



# Heterogeneity in Household Consumption Patterns (cont.)



## Hyperparameters

- ▶  $M = 5$
- ▶  $\underline{a}_1 = 10, \underline{a}_2 = 40$  (Dirichlet prior)
- ▶  $\underline{b}_1 = .5, \underline{b}_2 = .5$  (Gamma prior)

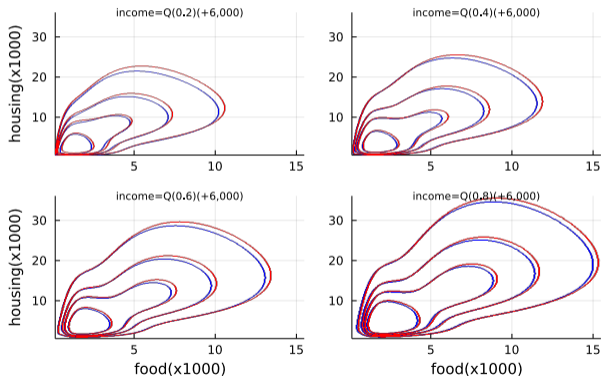
## MCMC samples

- ▶ Effective: 200,000 / 40  
(Burn-in: 400,000)

# Heterogeneity in Household Consumption Patterns (cont.)

Bivariate quantiles for food and housing conditional on four different income levels. Blue lines corr. to  $\alpha \in \{.2, .4, .6, .8\}$ .

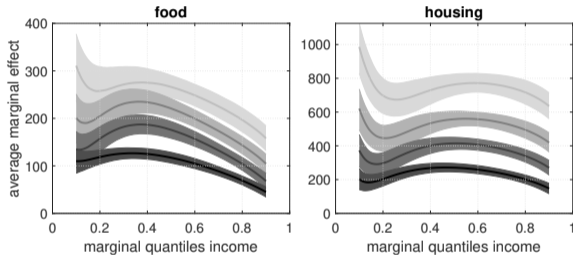
Red lines corr. to an income increase of \$6,000. QTE



- ▶ .2 expenditure quantile does not react considerably.
- ▶ .8 expenditure (.2 income) quantile substantially increases spending.
- ▶ No clear substitution patterns between food and housing.

# Heterogeneity in Household Consumption Patterns (cont.)

Quantile-varying marginal effects conditional on income.  
Shaded areas give the 90% C.I. for four income  $\alpha$ -levels.



- ▶ Low-income quantile households dedicate most of the additional income to food and shelter.
- ▶ Highest-income quantile households hardly increase spendings at all.

# Conclusion

Super-level sets provide a coherent framework for multivariate and univariate conditional as well as marginal quantiles:

- ▶ (1) no quantile crossing, (2) flexible quantile contours with exact probability coverage, (3) easy to extend quantile concept.

The overfitted GMM allows for straightforward incorporation of prior information regarding shapes and centers:

- ▶ enables a data driven bandwidth parameter selection without unpleasant computational features (slow convergence, long runtimes; Polonik, 1997).
- ▶ makes no particular residual distribution assumption (see, e.g., Sriram, Ramamoorthi & Ghosh (2013) on the invalidity of the  $\mathcal{AL}$ -likelihood).

Working paper available via  
<https://ideas.repec.org/p/tin/wpaper/20220094.html>

Many thanks for your attention!



# References

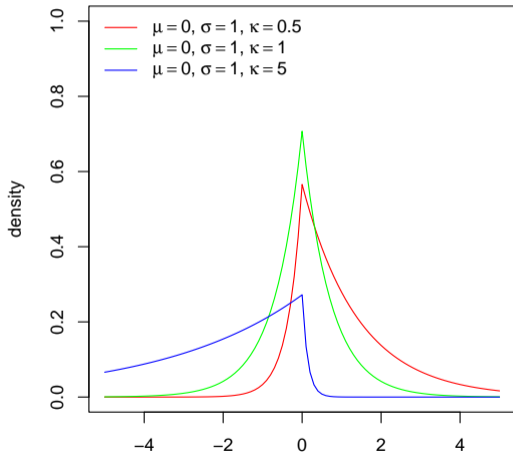
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# Asymmetric Laplace Distribution

Probability Function



# Prior Distributions

$$\boldsymbol{\mu}_m | \bar{\mathbf{v}}_0, \bar{\mathbf{V}}_0 \sim \mathcal{N}(\bar{\mathbf{v}}_0, \bar{\mathbf{V}}_0),$$

$$\bar{\mathbf{v}}_0 \sim \mathcal{N}(\underline{\mathbf{v}}, \underline{\mathbf{V}}),$$

$$\underline{\mathbf{v}} = \text{median}(\mathbf{y}_n), \underline{\mathbf{V}}^{-1} = \mathbf{0}$$

$$\bar{\mathbf{V}}_0 = \text{diag}(R_1^2 \lambda_1, \dots, R_K^2 \lambda_K),$$

$$\lambda_k \sim \mathcal{G}(\underline{b}_1, 1/\underline{b}_2).$$

with response variable-specific value ranges  $\{R_k\}$  and local shrinkage factors  $\{\lambda_k\}$  ( $\underline{b}_1, \underline{b}_2 > 0$ ).  
(see, Brown & Griffin, 2010)

$$\text{vec}(\mathbf{B}_m) \sim \mathcal{N}(\mathbf{c}_0, \mathbf{C}_0)$$

$$\boldsymbol{\Sigma}_m \sim \mathcal{IW}(\mathbf{S}_0, s_0)$$

where  $\mathbf{S}_0 = \mathbf{I}$  and  $s_0 > 2 + K$ .

# Sampling Algorithm

- ▶ Simulate mixture parameters conditional on  $\mathbf{z}_n$  ( $n = 1, \dots, N$ ,  $m = 1, \dots, M$ ):
  - ▶ Sample  $\{\kappa_m\}$  from  $\mathcal{D}(\bar{\rho}_1, \dots, \bar{\rho}_M)$  where  $\bar{\rho}_m = \rho_m + N_m$ ,  $N_m = \#\{n : z_n = m\}$ .
  - ▶ Sample  $\{\boldsymbol{\mu}_m\}$  from  $\mathcal{N}(\bar{\mathbf{v}}_m, \bar{\mathbf{V}}_m)$ .
  - ▶ Sample  $\{\mathbf{B}_m\}$  from  $\mathcal{N}(\mathbf{c}_m, \mathbf{C}_m)$ .
  - ▶ Sample  $\{\boldsymbol{\Sigma}_m\}$  from  $\mathcal{IW}(\mathbf{S}_m, s_m)$ .
- ▶ Sample  $z_n$  to classify observations conditional on mixture parameters ( $n = 1, \dots, N$ ):
  - ▶  $\pi_m \equiv \Pr[z_n = m | \mathbf{y}_m, \boldsymbol{\kappa}, \boldsymbol{\mu}, \mathbf{B}, \boldsymbol{\Sigma}] \propto \kappa_m \phi(\mathbf{y}_n; g_m(\mathbf{x}_n), \boldsymbol{\Sigma}_m)$ .
  - ▶ Sample  $\{z_n\}$  from  $\mathcal{M}(\pi_1, \dots, \pi_M)$ .
- ▶ Sample hyperparameters:
  - ▶ Sample  $\{\bar{\rho}_m\}$  simultaneously via a random walk MH-step with proposal density  $\log(\rho_m) \sim \mathcal{N}(\log(\rho_m), s_{\rho_m}^2)$  from  $p(\bar{\rho}_m | \boldsymbol{\kappa}) \propto p(\boldsymbol{\kappa} | \bar{\rho}_m) p(\bar{\rho}_m)$
  - ▶ Sample  $\{\lambda_k\}$  from  $\mathcal{GIG}(\underline{b}_1 - M/2, 2\underline{b}_2, \delta_k)$  where  $\delta_k = \sum_{m=1}^M (\mu_{m,k} - \bar{v}_{0,k})^2 / R_k^2$ .
  - ▶ Sample  $\bar{\mathbf{v}}_0$  from  $\mathcal{N}(\sum_{m=1}^M \boldsymbol{\mu}_k / M, \bar{\mathbf{V}}_0 / M)$  with  $\bar{\mathbf{V}}_0 = \text{diag}(R_1^2 \lambda_1, \dots, R_K^2 \lambda_K)$ .

# Super-level Set Algorithm

---

**Input** : chosen coverage probability  $\alpha$   
conditional distribution function  $F_{\mathbf{Y}_{\mathcal{K}}|\mathbf{Y}_C=\mathbf{y}_C}(\mathbf{y})$   
grid boundary probability  $\epsilon$   
dimension-specific grid point number  $n_{\text{grid}}$

**Output:** actual coverage probability  $p$   
numerical quantile  $\tilde{Q} = \tilde{Q}_{\mathbf{Y}_{\mathcal{K}}|\mathbf{Y}_C=\mathbf{y}_C}(\alpha)$  of size  $n_{\text{grid}}^{|\mathcal{K}|}$

```
1 for  $k \in \mathcal{K}$  do
2   grid $k$  = equally spaced  $n_{\text{grid}}$  vector with values
   from  $F_{Y_k|\mathbf{Y}_C=\mathbf{y}_C}^{-1}(\epsilon)$  to  $F_{Y_k|\mathbf{Y}_C=\mathbf{y}_C}^{-1}(1 - \epsilon)$ ;
3    $\tilde{Q}_{\mathbf{Y}_{\mathcal{K}}|\mathbf{Y}_C=\mathbf{y}_C}(\alpha) = |\mathcal{K}|$ -dimensional array of zeros
4    $P =$  empty  $|\mathcal{K}|$ -dimensional array to hold probabilities per hypercube
5   for  $(i_1 \in 2 : n_{\text{grid}}), (i_2 \in 2 : n_{\text{grid}}), \dots, (i_{|\mathcal{K}|} \in 2 : n_{\text{grid}})$  do
6      $P_{i_1, i_2, \dots, i_{|\mathcal{K}|}} = \Pr[Y_k \in [\text{grid}_{k, i_k - 1}, \text{grid}_{k, i_k}] \forall k \in \mathcal{K} | \mathbf{Y}_C = \mathbf{y}_C]$ 
7    $p = 0$ 
8   while  $p < \alpha$  do
9      $\mathcal{I} =$  set of indices for which  $P$  equals  $\max\{P\}$ 
10     $p = p + \sum_{i \in \mathcal{I}} P_i$ 
11    for  $i \in \mathcal{I}$  do
12       $\tilde{Q}_i = \alpha$ 
13       $P_i = 0$ 
```

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# Quantile-Specific Measures

The local marginal effect in the  $\alpha$ -level quantile of  $Y_k$  given  $\mathbf{Y}_C = \mathbf{y}_C$  for a change from  $\mathbf{x}$  to  $\mathbf{x} + \Delta_g$  is:

$$\beta_{k|C}^g(\alpha|\mathbf{y}_C, \mathbf{x}) = Q_{Y_k|Y_C=\mathbf{y}_C}(\alpha|\mathbf{x} + \Delta_g) - Q_{Y_k|Y_C=\mathbf{y}_C}(\alpha|\mathbf{x}),$$

where  $\Delta_g$  is a vector with a small value  $\delta_g$  at position  $g$  and zeros elsewhere (see Doksum, 1974). [Back](#)

# Data Generating Processes

1 Multivariate Gaussian:

$$\mathbf{y}_n \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \text{ with } \boldsymbol{\mu} = [.2, .2, .2]' \text{ and } \Sigma_{jj} = .4, \Sigma_{jk} = .25 (\forall j \neq k).$$

2 Multivariate Student-t:

$$\mathbf{y}_n \sim t_r(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \text{ with } r = 5, \boldsymbol{\mu} = [.2, .2, .2]' \text{ and } \Sigma_{jj} = .4, \Sigma_{jk} = .25 (\forall j \neq k).$$

3 Multivariate log-Gaussian:

$$\mathbf{y}_n \sim \log \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \text{ with } \boldsymbol{\mu} = [.2, .2, .2]' \text{ and } \Sigma_{jj} = .4, \Sigma_{jk} = .25 (\forall j \neq k).$$

4 Conditional heteroskedasticity:

$$\mathbf{y}_n \sim \mathcal{N}(\boldsymbol{\mu}, \Omega_n) \text{ with } \boldsymbol{\mu} = [.2, .2, .2]' \text{ and } \Omega_n = \exp(z_n)\boldsymbol{\Sigma} \text{ where } z_n \sim \mathcal{N}(0, 1) \text{ and } \Sigma_{jj} = .4, \Sigma_{jk} = .25, \forall j \neq k.$$

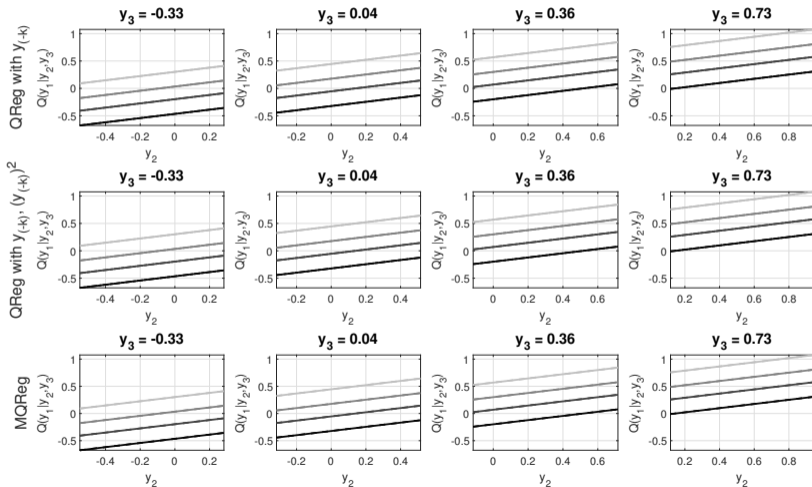
5 Multivariate Gaussian mixture:

$$\mathbf{y}_n \sim \mathcal{N}(\boldsymbol{\mu}_{z_n}, \boldsymbol{\Sigma}_{z_n}) \text{ with } \Pr[z_n = m] = .33, \text{ for } m = 1, 2, 3, \boldsymbol{\mu}_1 = [2, 2, 2], \boldsymbol{\mu}_2 = [0, 0, 0], \boldsymbol{\mu}_3 = [-2, .5, 1] \text{ and } \Sigma_{1,jj} = .4, \Sigma_{1,jk} = .25, \boldsymbol{\Sigma}_2 = \mathbf{I}, \Sigma_{3,jj} = .7, \Sigma_{3,jk} = .5.$$



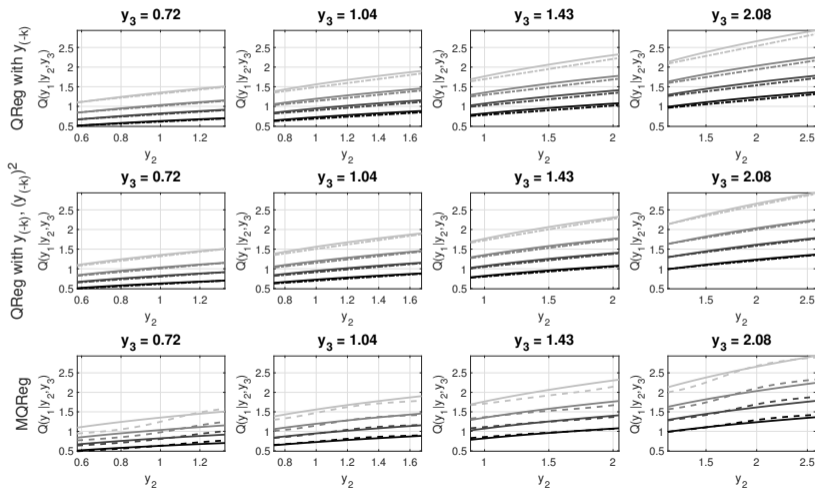
# Simulation Exercise: Multivariate Gaussian

Estimated (dashed lines) vs. true (solid lines) conditional quantiles for  $\alpha \in \{.2, .4, .6, .8\}$



# Simulation Exercise: Multivariate Student-t

Estimated (dashed lines) vs. true (solid lines) conditional quantiles for  $\alpha \in \{.2, .4, .6, .8\}$



# Simulation Exercise: Multivariate log-Gaussian

Estimated (dashed lines) vs. true (solid lines) conditional quantiles for  $\alpha \in \{.2, .4, .6, .8\}$

