One-day course on symmetry-modulated distributions

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Skewed world of data: Workshop in honor of Reinaldo B. Arellano-Valle's 65th birthday October 2017 Pontificia Universidad Católica de Chile

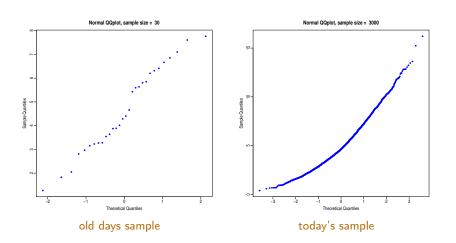
Prólogos

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Lots of distributions available, do we need more?

- Probability textbooks introduce 'standard' distributions
- Over the years many others have been introduced
- Classical work includes proposals by K.Pearson, Fechner, Edgeworth, Johnson, Burr, etc.
- Still the search keeps going.
- Two currently popular general approaches: ('general': allowing unlimited number of specific constructions)
 - copulae
 - symmetry-modulated distributions, AKA skew-symmetric distributions
- Question: why so much effort?

Illustration: QQ-normal probability plots from two samples



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Larger datasets require more accurate modelling

- The two datasets are sampled from the same distribution
- The visual message of normal QQ-plot is completely different
- although only the sample size has changed
- Only the larger sample could highlight non-normality
- Today larger and larger datasets are available
- More data is good, but also more challenging
- We need flexible tools for accurate modelling of large datasets

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Multivariate datasets are increasingly more frequent

- data collection is more often multivariate, possibly highly so
- many above-quoted formulations are univariate
- special interest in developing flexible multivariate distributions
- ... flexible yet mathematically tractable

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Our plan of work

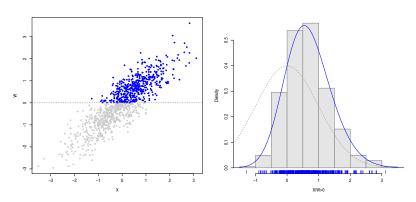
A tutorial to symmetry-modulated distributions:

- introduce main concepts in the univariate case
- focus on key special cases
- extend concepts to the multivariate settings
- sketch of some extensions
- followed by practical work with R package 'sn'

Básis (
$$d=1$$
)

Skew-normal distribution - idea

Idea: start from a normal distribution and 'perturb' it. Perturbation, or modulation, is achieved by a selection mechanism.



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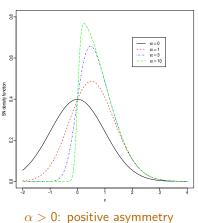
Skew-normal distribution – compute density function

assume :
$$(X,W) \sim \mathrm{N}_2(0,\Sigma), \qquad \Sigma = \begin{pmatrix} 1 & \delta \\ \delta & 1 \end{pmatrix}$$
 recall : $(W|X=x) \sim \mathcal{N}(\delta x, 1-\delta^2)$ (density at $x|W \geq 0$) = $\frac{1}{\mathrm{d}x} \mathbb{P}\{X \in (x,x+\mathrm{d}x)|W \geq 0\}$ = $\frac{1}{\mathrm{d}x} \frac{\mathbb{P}\{X \in (x,x+\mathrm{d}x) \cap W \geq 0\}}{\mathbb{P}\{W \geq 0\}}$ = $\frac{1}{\mathrm{d}x} \frac{\mathbb{P}\{X \in (x,x+\mathrm{d}x)\} \mathbb{P}\{W \geq 0|X=x\}}{1/2}$ = $\frac{2}{\mathrm{d}x} \frac{\varphi(x) \Phi(\alpha x), \qquad \alpha = \frac{\delta}{\sqrt{1-\delta^2}} \in \mathbb{R}$

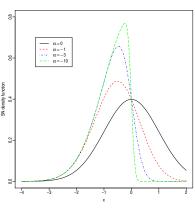
write : $Z \equiv (X|W > 0) \sim SN(\alpha)$

Básis (d=1)Plus (d = 1)Básis (d > 1)

Skew-normal distribution – density function plots



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 α < 0: negative asymmetry $\alpha = 0$: null asymmetry, i.e. N(0,1) $\alpha = 0$: null asymmetry, i.e. N(0,1)

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Towards a general result, preliminaries

- let $(X, W) \sim N_2(0, \Sigma)$ as before
- $T = -(W \delta X)/\sqrt{1 \delta^2} \sim N(0, 1)$
- $cov{X, T} = 0 \implies X \perp \!\!\!\perp T \text{ (independent)}$
- $(W \ge 0)$ is algebraically equivalent to $(T \le \alpha X)$
- hence $Z \equiv (X|W \ge 0) \equiv (X|T \le \alpha X)$
- Note the key ingredients here: $X \perp \!\!\! \perp T$, X and T symmetric about 0, and so is $T \alpha X$

A general result

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Lemma (Univariate version)

If f_0 is PDF and G_0 a continuous CDF on \mathbb{R} , both symmetric about 0, then

$$f(x) = 2 f_0(x) G_0\{w(x)\}, \qquad x \in \mathbb{R},$$

is a proper density function for any odd function w.

Proof. Denote $X \sim f_0$ and $T \sim G_0$, independent rv's. The distribution of T - w(X) is symmetric about 0. Then

$$\frac{1}{2} = \mathbb{P} \{ T - w(X) \le 0 \}
= \mathbb{E}_X \{ \mathbb{P} \{ T \le w(x) | X = x \} \}
= \int_{\mathbb{R}} G_0 \{ w(x) \} f_0(x) dx$$

Some comments

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- Above result allows to combine freely f_0 , G_0 and w: a huge variety of constructions are possible
- however, 'possible' does not automatically imply 'useful': need to select those which are worth of consideration
- ullet The result works also if the support is a subset of ${\mathbb R}$
- The lemma allows a number of extensions: multivariate, non-odd w, discrete variables, etc. (Some of these extensions will be examined later)
- From the assumptions of the lemma, $G(x) = G_0\{w(x)\}$ satisfies

$$G(x) \ge 0,$$
 $G(x) + G(-x) = 1.$

Possible to formulate the result equivalently in terms of G(x).

Crude version Generate $X \sim f_0$ and $T \sim G_0$ independently and set

$$Z = (X | T \le w(X))$$

Drawback: reject sampled values with T > w(X), half of them on average.

Improved version

$$Z = \begin{cases} X & \text{if } T \le w(X) \\ -X & \text{otherwise} \end{cases}$$

No rejection of sampled values

Perturbation invariance

• Recall stochastic representation

$$Z = \begin{cases} X & \text{if } T \le w(X) \\ -X & \text{otherwise} \end{cases}$$

- then |Z| is distributed like |X|, write $|Z| \stackrel{d}{=} |X|$
- more generally: $t(Z) \stackrel{d}{=} t(X)$ for any even $t(\cdot)$ \Rightarrow property of perturbation (or modulation) invariance
- Example: if $Z \sim SN(\alpha)$, then $Z^2 \sim \chi_1^2$

Plus
$$(d=1)$$

More on SN: other stochastic representations

Representation by conditioning/selection this was how we introduced the SN distribution

Additive representation

- If $U_0,\,U_1$ are independent $\mathrm{N}(0,1)$ variables, then $Z = \sqrt{1-\delta^2}\;U_0 + \delta\,|U_1| \sim \mathrm{SN}(\alpha)$
- much used to develop EM-type algoritms

Representation via minima/maxima

- assume (X, Y) is bivariate standard Normal with $corr\{X, Y\} = \rho$
- write $\alpha = \sqrt{(1-\rho)/(1+\rho)}$
- then $\max(X,Y) \sim \mathrm{SN}(\alpha)$ and $\min(X,Y) \sim \mathrm{SN}(-\alpha)$

More on SN: some formal properties

• Moment generating function has a simple expression:

$$M(t) = 2 \exp(\frac{1}{2}t^2) \Phi(\delta t)$$

 \implies can compute moments

e.g.
$$\mathbb{E}{Z} = \sqrt{\frac{2}{\pi}} \delta = \sqrt{\frac{2}{\pi}} \frac{\alpha}{\sqrt{1+\alpha^2}}$$

(only odd moments are necessary)

⇒ derive futher properties

e.g. if
$$Z \sim \mathrm{SN}(\alpha) \perp \!\!\!\perp U \sim \mathrm{N}(0,1)$$
, $Z + U \sim \sqrt{2} \times \mathrm{SN}(\tilde{\alpha})$

• Distribution function has a tractable expression

SN: about tails

consider ratio of SN vs N tails:

$$\operatorname{ratio}(x) = \frac{2 \varphi(x) \Phi(\alpha x)}{\varphi(x)}$$
 as $x \to \pm \infty$

• if $\alpha > 0$,

$$ratio(x) = 2 \Phi(\alpha x) \to \begin{cases} 2 & \text{if } x \to +\infty \\ 0 & \text{if } x \to -\infty \end{cases}$$

if $\alpha <$ 0, just swap $\pm \infty$

- Implication: tails decay either at the same rate of N(0,1) or faster
- Same conclusion if SN density is replaced by another one like

$$f(x) = 2 \varphi(x) G_0(\alpha x)$$

Thick tails

- In many situation we need thicker-than-normal tails (occasionally need thinner-than-normal tails)
- This feature cannot be achieved by perturbation of N(0,1)
- We must start from a baseline density f_0 in

$$f(x) = 2 f_0(x) G_0\{w(x)\}$$

which already has thick tails

- Many possible options
- Preference for those where f₀ allows a tail-regulation parameter

Skew-t (ST) distribution – genesis

- A good choice for f_0 is the Student's t density: $t(x; \nu)$, $\nu > 0$
- Even then, still many possible options, such as the 'linear form'

$$2 t(x; \nu) T(\alpha x; \nu)$$

- There are strong reasons for picking up another option
- Recall origin of classical Student's t:

$$Z \sim \mathrm{N}(0,1) \perp \!\!\! \perp W_{
u} \sim \chi_{
u}^2 \quad \Longrightarrow \quad \left| \frac{Z}{\sqrt{W_{
u}/
u}} \sim t(x;
u) \right|$$

- Use the the same construction with $Z \sim SN(\alpha)$ \implies obtain the $ST(\alpha, \nu)$ distribution
- Note: the link with the classical $t(x; \nu)$ is not the only reason
- Beware: in literature various other proposals named 'skew-t'

Skew-t (ST) distribution – a closer look

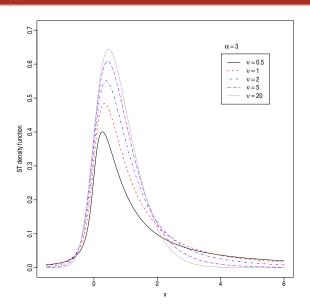
• Algebraic work leads to $ST(\alpha, \nu)$ density function:

$$2 t(x; \nu) T\left(\alpha x \sqrt{\frac{\nu+1}{\nu+x^2}}; \nu+1\right)$$

- $Z \sim ST(\alpha, \nu) \implies Z^2 \sim F(1, \nu)$
- m-th order moment exist if $m < \nu$, like regular t
- explicit expressions available up to m = 4
 (if necessary, higher moments could be worked out)
- a very wide range of γ_1 (skewness) and γ_2 (kurtosis) $-\infty < \gamma_1 < \infty, \qquad 0 \le \gamma_2 < \infty \qquad \text{(but no } \gamma_2 < 0 \text{)}$
- widely flexible shape, well-suited for data fitting (when complemented with location and scale parameters)
- as $\nu \to \infty$, density $ST(\alpha, \nu) \to SN(\alpha)$

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Skew-t (ST) distribution – examples of density



Data

- Let Z be a SN or ST or something-of-the-kind random variable
- For applied work, introduce location and scale parameters:

$$Y = \xi + \omega Z, \qquad \xi \in \mathbb{R}, \quad \omega \in \mathbb{R}^+$$

- correspondingly extend our notation to $Y \sim SN(\xi, \omega, \alpha)$ and $Y \sim ST(\xi, \omega, \alpha, \nu)$
- Note: ξ is not the mean, ω is not the standard deviation (this is why we do not use classical μ, σ symbols)

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Fitting a SN distribution

- Start from simple case of i.i.d. observations $y = (y_1, \dots, y_n)$
- log-likelihood for SN:

$$\log L(\xi, \omega, \alpha) = \operatorname{constant} - \frac{1}{2} n \log \omega - \frac{1}{2} \sum_{i} z_{i}^{2} + \sum_{i} \log \Phi(\alpha z_{i})$$
having set
$$z_{i} = (y_{i} - \xi)/\omega$$

• In a regression model, location depends on covariates x_i , typically in a linear form:

$$\xi_i = \mathbf{x}_i^{\mathsf{T}} \boldsymbol{\beta}$$
 $\mathbf{x}_i, \boldsymbol{\beta} \in \mathbb{R}^p, \quad i = 1, \dots, n$

• log-likelihood log $L(\beta, \omega, \alpha)$ is as before, except that now

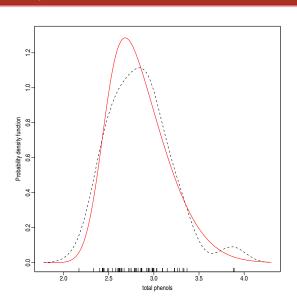
$$z_i = (y_i - \xi_i)/\omega = (y_i - x_i^{\top} \beta)/\omega$$

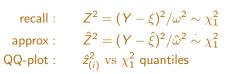
Illustration: fitting SN to phenols content in Barolo wine

$$n = 59$$

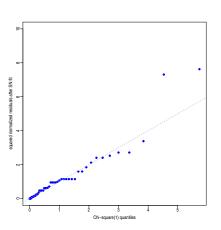
$$\hat{\gamma}_1 = 0.8$$

$$\frac{\hat{\gamma}_1}{\text{std.err.}} = 2.5$$





with ST: replace χ_1^2 with $F(1, \hat{\nu})$



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SN log-likelihood: some unusual aspects

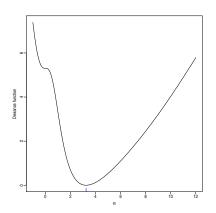
Two sort of noteworthy phenomena

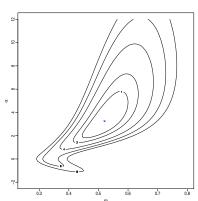
- 'Transient' sort of occasional events
 Usually with small n, sporadic if n beyond a few dozens
 Similar behaviour fairly common also with other models
 - multiple local maxima
 - max log L occurs at $\alpha \to \pm \infty$
- 'Persistent (but local)' behaviour: that is, for all samples, but only at $\alpha = 0$
 - stationarity of log L at point $\alpha = 0$
 - correspondingly, singularity of the information matrix

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SN log-likelihood: stationarity of log L at $\alpha = 0$

deviance (LRT) : $D(\theta) = 2 \{ \log L(\hat{\theta}) - \log L(\theta) \}$ profile deviance : $D(\theta) = 2 \{ \log L(\hat{\theta}, \hat{\psi}) - \log L(\theta, \hat{\psi}(\theta)) \}$





CP for SN

- The twists of $\log L$ at $\alpha=0$ can be fixed by switching from 'direct' (DP) to 'centred parameterization' (DP)
- Conceptually, we re-parameterize as

$$Y = \xi + \omega Z = \mu + \sigma Z_0$$

via the 'centred variable'

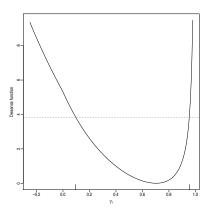
$$Z_0 = (Z - \mathbb{E}\{Z\})/\mathrm{std.dev.}(Z)$$

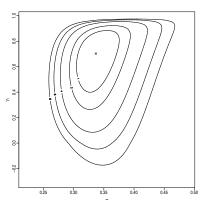
- $CP = (\mu, \sigma, \gamma_1)$
- In parallel, CP avoids singularity of the information matrix
- Importantly, CP is easier to interpret than DP

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SN log-likelihood: using CP with the Barolo data

deviance (LRT) : $D(\theta) = 2 \{ \log L(\hat{\theta}) - \log L(\theta) \}$ profile deviance : $D(\theta) = 2 \{ \log L(\hat{\theta}, \hat{\psi}) - \log L(\theta, \hat{\psi}(\theta)) \}$





- With ST model no stationarity of log L at $\alpha = 0$
- hence no singularity of information matrix at $\alpha = 0$
- \bullet in fact, these issues are specific 'only' of φ baseline
- still CP useful for easier interpretability

Multivariate skew-normal distribution: genesis

ullet SN was constructed from bivariate standard normal (X,W) as

$$Z = (X|W \ge 0)$$

• Now start from (d+1)-dimensional Normal with std margianle

$$egin{array}{l} d & X \\ 1 & W \end{array} \sim \mathrm{N}_{d+1}(0,ar{\Sigma})$$

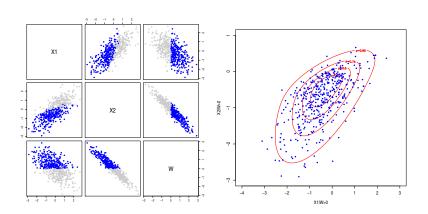
where $\bar{\Sigma}$ is a correlation matrix

$$ar{\Sigma} = egin{pmatrix} ar{\Omega} & \delta \ \delta^ op & 1 \end{pmatrix}$$

• and then use the same conditioning process: $Z = (X|W \ge 0)$ except that now X is d-dimensional

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Multivariate SN – illustration of genesis



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Multivariate SN — basic formal facts

• If $Z = (X|W \ge 0)$, its density function turns out to be:

$$2 \varphi_d(x; \bar{\Omega}) \Phi(\alpha^\top x), \qquad x \in \mathbb{R}^d,$$

where $\varphi_d(x; V)$ is $N_d(0, V)$ density and

$$\alpha = \left(1 - \delta^{\top} \bar{\Omega}^{-1} \delta\right)^{-1/2} \bar{\Omega}^{-1} \delta \in \mathbb{R}^d$$

Moment generating function has a simple expression:

$$M(t) = 2 \exp(\frac{1}{2}t^{\top}\bar{\Omega}^{\top}t) \Phi(\delta^{\top}t)$$

- \implies can compute moments, e.g. $\mathbb{E}\{Z\} = \sqrt{2/\pi} \,\delta$ ⇒ derive further properties
- Additive representation extends to multivariate SN:

$$Z = \left(I_d - \operatorname{diag}(\delta)^2\right)^{1/2} U_0 + \delta |U_1|$$

where $U_0 \sim N_d(0, \Psi) \perp U_1 \sim N(0, 1)$.

Multivariate SN — include location and scale

- Start from $Z = (Z_1, \dots, Z_d)^{\top}$ with density $2 \varphi_d(x; \bar{\Omega}) \Phi(\alpha^{\top} x)$
- introduce location and scale:

$$\begin{pmatrix} Y_1 \\ \vdots \\ Y_d \end{pmatrix} = \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_d \end{pmatrix} + \begin{pmatrix} \omega_1 & 0 \\ & \ddots & \\ 0 & \omega_d \end{pmatrix} \begin{pmatrix} Z_1 \\ \vdots \\ Z_d \end{pmatrix}$$

write more compactly

$$Y = \xi + \omega Z$$

where $\omega = \operatorname{diag}(\omega_1, \ldots, \omega_d)$

- notation: $Y \sim \mathrm{SN}_{d}(\xi, \Omega, \alpha)$ where $\Omega = \omega \; \bar{\Omega} \; \omega$
- density at $x \in \mathbb{R}^d$:

$$2 \varphi_d(x - \xi; \Omega) \Phi(\alpha \omega^{-1}(x - \xi))$$

Recall elliptical families

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- Recall continuous elliptically contoured (EC) distributions
- Density constant on ellipsoids:

$$f(x) = \frac{c_d}{(\det \Sigma)^{1/2}} g_d \left((x - \mu)^\top \Sigma^{-1} (x - \mu) \right), \qquad x \in \mathbb{R}^d$$

- Notation: $X \sim \mathrm{EC}_d(\mu, \Sigma, g_d)$
- density is centrally symmetric about μ : $f(x \mu) = f(\mu x)$
- Extends the normal distribution which corresponds to

$$g_d(u) = \exp(-u/2)$$

- The key aspect is that the EC family encompasses many others
- and it still preserves various properties of normal distribution:
 - family closed under marginalization
 - family closed under conditioning
 - conditional mean is linear function of the conditioning variables
- An interesting case is the multivariate Student's t:

$$g_d(u) = (1 + u/\nu)^{-(d+\nu)/2}$$

Skew-elliptical distributions

Start from

$$\begin{pmatrix} X \\ W \end{pmatrix} \sim \mathrm{EC}_{d+1}(0, \bar{\Sigma}, g_{d+1})$$

• and apply the 'usual' conditioning (or selection) process:

$$Z = (X|W > 0)$$

- Introduce location and scale: $Y = \xi + \omega Z$
- Terminology: Y and Z have skew-elliptical distribution (SEC)
- If (X, W) is normal, reproduce $Y \sim SN_d(\xi, \Omega, \alpha)$
- Another noteworthy case with $(X, W) \sim t_{d+1}(0, \bar{\Sigma}, \nu)$:

$$Y \sim \mathrm{ST}_d(\xi, \Omega, \alpha, \nu)$$

• density of normalized r.v. $Z \sim \mathrm{ST}_d(0, \bar{\Omega}, \alpha, \nu)$:

$$2: t_d(z; \bar{\Omega}) \ T\left(\alpha^\top z \sqrt{\frac{\nu + d}{\nu + z^\top \bar{\Omega}^{-1} z}}; \nu + d\right), \qquad z \in \mathbb{R}^d$$

A general result

Lemma (Multivariate version)

If f_0 is a PDF on \mathbb{R}^d and G_0 a continuous CDF on \mathbb{R} , both symmetric about 0, then

$$f(x) = 2 f_0(x) G_0\{w(x)\}, \qquad x \in \mathbb{R}^d,$$

is a proper density function for any odd function $w(\cdot)$ on \mathbb{R}^d .

Proof: a simple extension of the univariate version.

Notes:

- (1) f_0 symmetric on \mathbb{R}^d means $f_0(x) = f_0(-x)$ for all $x \in \mathbb{R}^d$
- (2) w odd function on \mathbb{R}^d means w(-x) = -w(x) for all $x \in \mathbb{R}^d$.

A general result — comments

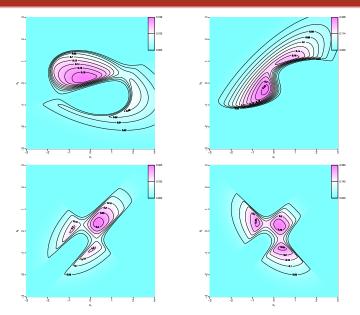
- Both SN_d and ST_d have density like f(x) in the lemma
- Can show that all SEC distributions have this structure with 'baseline density' f_0 of elliptical type
- But the lemma allows f_0 to be non-elliptical and G_0 can be unrelated to f_0 , unlike in SEC's
- This modulation process can produce all sort of shapes, even guite bizarre ones, not just 'skew'
- Next plots illustrate this point using

$$f_0 = \varphi_2, \qquad G_0 = \Phi$$

$$w(x_1, x_2) = a_1 x_1 + a_2 x_2 + a_3 x_1^3 + a_4 x_2^3 + a_5 x_1^2 x_2 + a_6 x_1 x_2^2$$

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Examples of modulated bivariate normal densities



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Some formal properties of the general constuction

$$f(x) = 2 f_0(x) G_0\{w(x)\}, \qquad x \in \mathbb{R}^d$$

Stochastic representation If $X \sim f_0 \perp \!\!\! \perp T \sim G_0$, then

$$Z = \begin{cases} X & \text{if } T \leq w(X) \\ -X & \text{otherwise} \end{cases}$$
 has density $f(\cdot)$

Perturbation (or modulation) invariance Now holds multivariate:

$$t(Z) \stackrel{d}{=} t(X)$$

for any even t(x), mapping $\mathbb{R}^d \to \mathbb{R}^q$

Examples If $Y \sim SN_d(\xi, \Omega, \alpha)$ and $V \sim ST_d(\xi, \Omega, \alpha, \nu)$, then $(Y-\xi)^{\top}\Omega^{-1}(Y-\xi) \sim \chi^2_{A}$ $(V-\varepsilon)^{\top}\Omega^{-1}(V-\varepsilon) \sim d \times F(d,\nu)$

These facts are useful for model diagnostics.

Many additional developments

- Many forms of generalization exist
- The more tractable case is the extended SN and alike: start from $(X, W) \sim N_2$ and take $(X|W \ge c)$ with $c \in \mathbb{R}$
- Important extension: m-dimentional conditioning variable W
 relatively tractable in normal context (Closed SN)
 to some extent also tractable in EC class
- General selection mechanism: replace $(\cdots|W\geq 0)$ by $(\cdots|W\in C)$ with $C\subset\mathbb{R}^m$ (For general C, difficult to find normalizing constant)

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Use in statistical methods and applied areas

Two intersecting levels of work:

- Extensions of standard statistical methods
- Application in diverse fields, often with suitable methodological adaption of existing techniques

Many domains:

- classical areas of statistical methods, such as longitudinal data, factor analysis, item response analysis, . . .
- much impact especially in model-based clustering
- flexible distributions provide a route to robustness
- much work in finance, theoretical and empirical
- but also in environmental risk, medical statistics, econometrics, income distribution, data confidentiality, insurance, industrial statistics and reliability, cell biology, forestry, et cetera...

Any future?

- Formidable work has been deployed, but still room for progress
- Extension of standard statistical methods for more flexible models, with applications
- Futher advances possible in the study of flexible distributions (a personal view presented in more specialized topic session)

Ultra

Ω

Resources

A complete list of references would take many pages. An absolutely minimal list is:

- A Azzalini & A Capitanio (2014), monograph, Cambridge UP
- MG Genton (2004), edited volume, C&H/CRC
- R software: https://cran.r-project.org/package=sn