

# Anomaly detection using surprisals

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# Outline

- 1 Anomalies and surprisals
- 2 Extreme value theory and surprisals
- 3 Lookout algorithm
- 4 Conclusions

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1 Anomalies and surprisals

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# Definitions of anomalies

*an observation (or a subset of observations) which appears to be inconsistent with the remainder of that set of data.*

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*an observation which deviates so much from other observations as to arouse suspicion it was generated by a different mechanism.*

(Hawkins, 1980)

# Definitions of anomalies

## Definition: Anomaly

Given a set of observations  $\{y_1, \dots, y_n\}$  drawn from probability distribution  $F$ ,  $y_i$  is an **anomaly** if

$$\mathbb{P}(f(Y) < f(y_i)) < \alpha$$

where  $Y \sim F$ ,  $f$  is the generalized density of  $F$ , and  $\alpha > 0$  is a chosen threshold.

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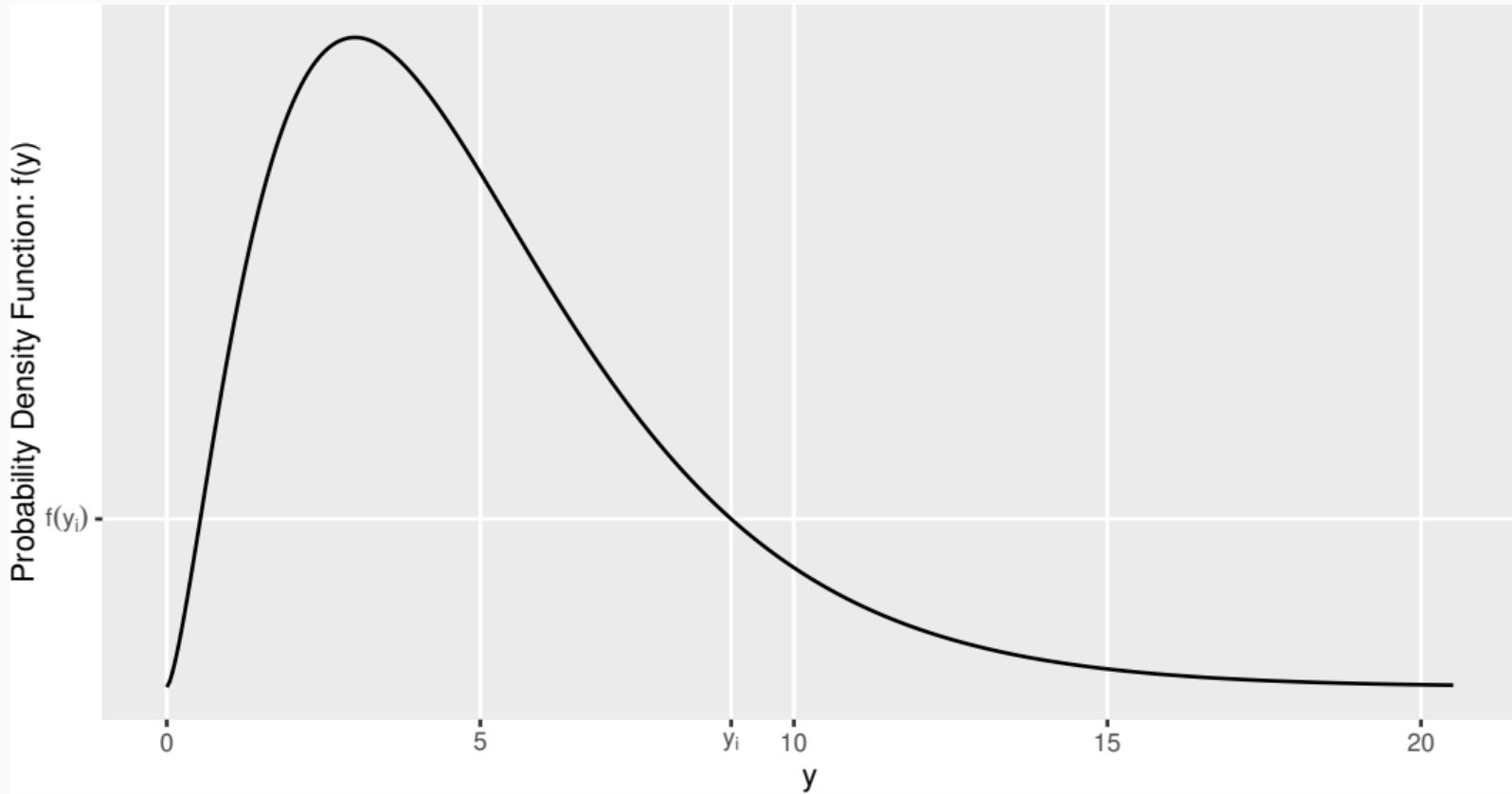
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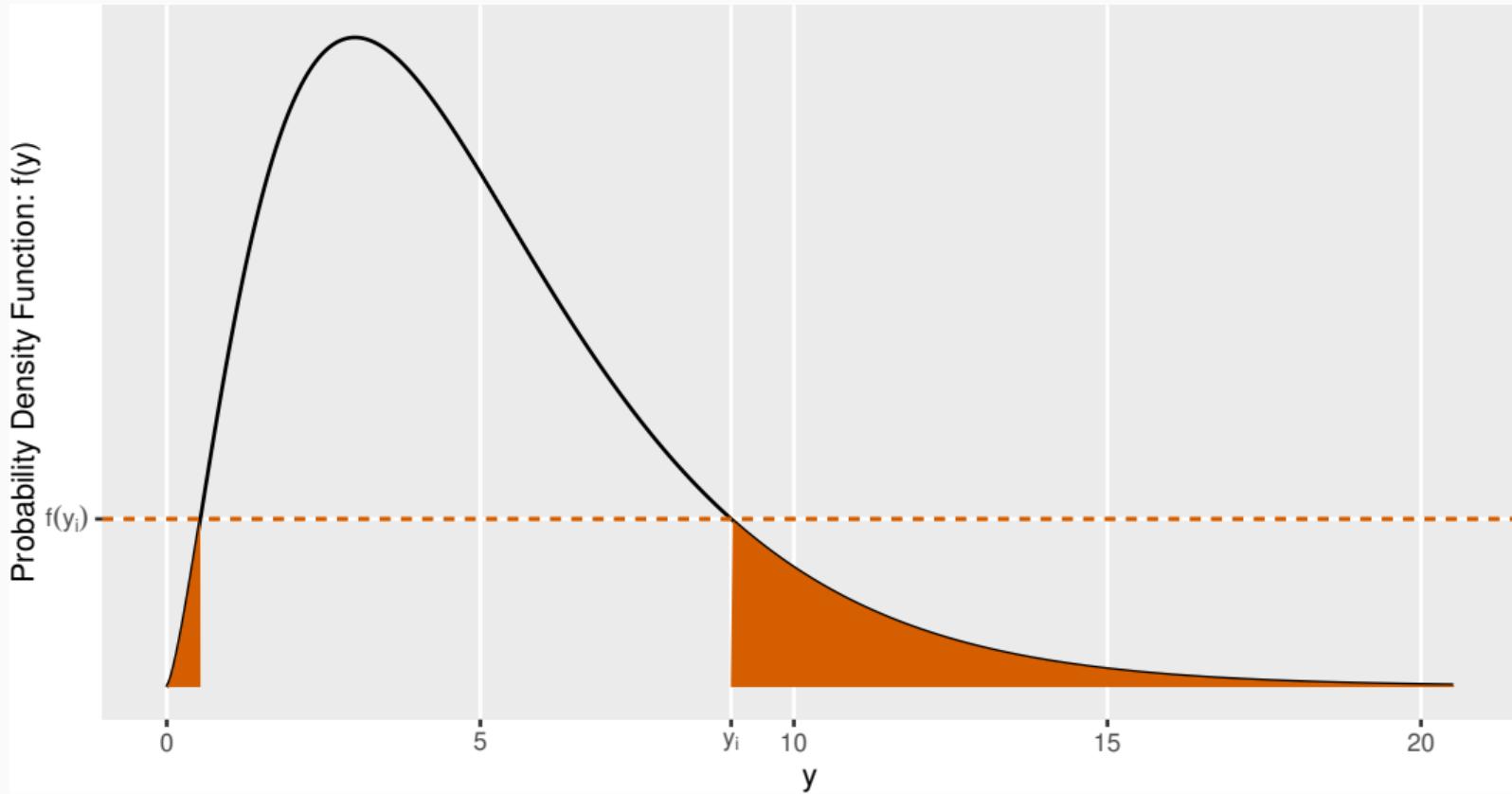
where  $Y \sim F$ ,  $f$  is the generalized density of  $F$ , and  $\alpha > 0$  is a chosen threshold.

- $y_i$  can be a scalar, vector or a more complex object
- $f$  can be a conditional density, and can be known or estimated

# Definitions of anomalies



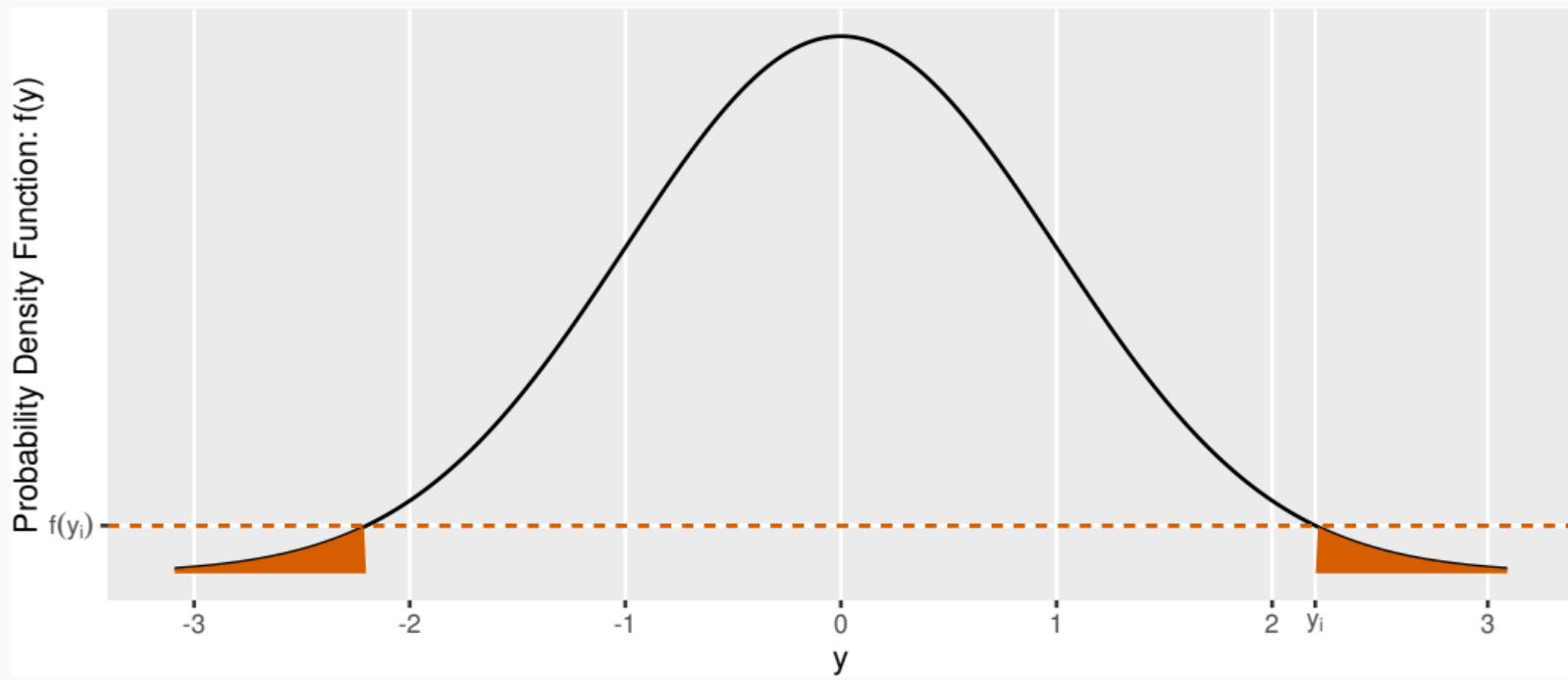
# Definitions of anomalies



# Anomaly detection: Normal distribution

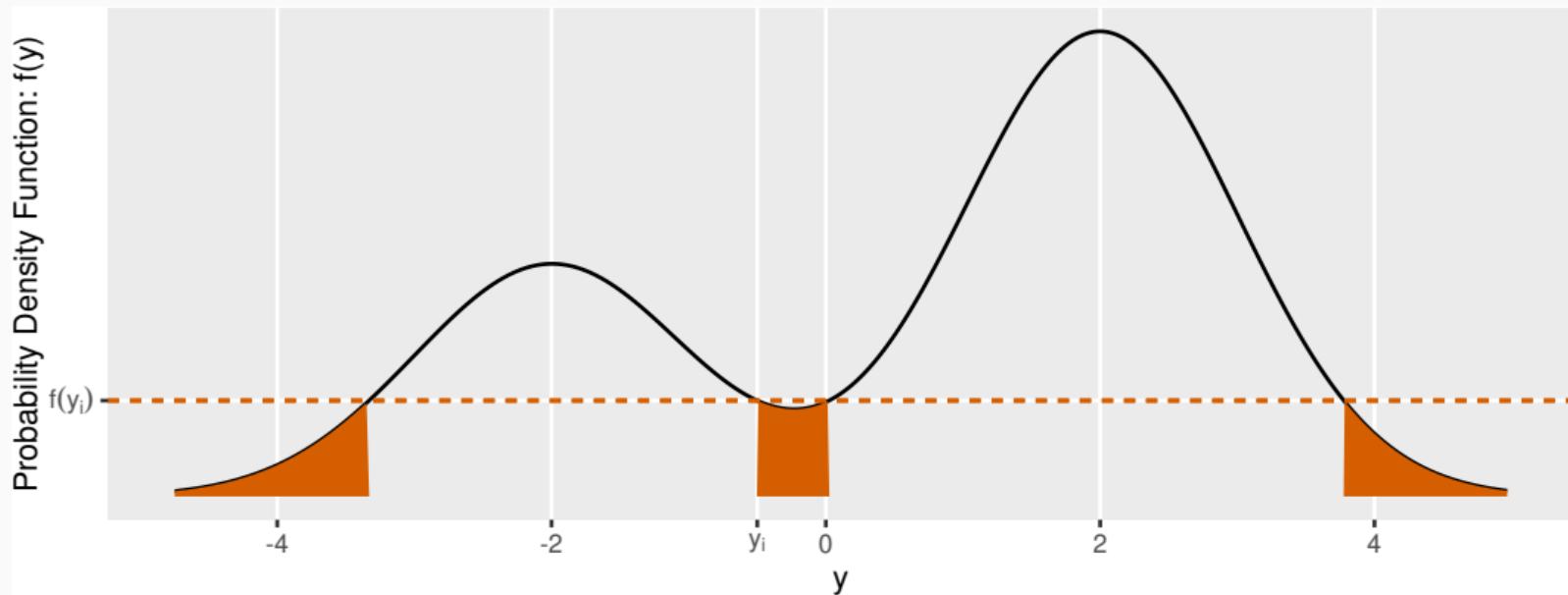
If  $F \sim N(\mu, \sigma^2)$ , then  $p_i = 2 [1 - \Phi(|y_i - \mu|/\sigma)]$

Equivalent to a two-sided p-value from a z-score test.



# Anomaly detection: Highest density regions

HDR with probability  $1 - \alpha$  is  $R_\alpha = \{y : f(y) \geq c_\alpha\}$  where  $c_\alpha$  is largest constant s.t.  $\mathbb{P}(Y \in R_\alpha) \geq 1 - \alpha$ .  
An observation is an anomaly if  $y_i \notin R_\alpha$ .



# Surprises

## Definition: Surprisal

The **surprisal** of an observation  $y_i$  drawn from probability distribution  $F$  with generalized density  $f$  is defined as

$$s_i = -\log f(y_i)$$

- Better known as “log scores” in statistics.
- “Surprisal” coined by Tribus (1961).
- Average surprisal = entropy of random variable
- Sum of surprisals = negative log likelihood

# Anomaly detection using surprisals

Let  $G(s) = \mathbb{P}(S \leq s)$  be the **surprisal distribution** where  $S = -\log f(Y)$  and  $Y \sim F$ .

$$G(s) = \mathbb{P}(-\log f(Y) \leq s) = \mathbb{P}(f(Y) \geq e^{-s})$$

The **surprisal score** is

$$p_i = 1 - G(s_i)$$

and an observation is an **anomaly** if  $p_i < \alpha$ .

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# Fisher-Tippett-Gnedenko theorem

Consider  $n$  iid rvs  $S_1, \dots, S_n$  with cdf  $G$  and  $M_n = \max\{S_1, \dots, S_n\}$ . If there exist sequences of constants  $\{a_n > 0\}$  and  $\{b_n\}$  such that

$$\mathbb{P}\left\{(M_n - b_n)/a_n \leq z\right\} \rightarrow H(z) \quad \text{as } n \rightarrow \infty,$$

for a non-degenerate cdf  $H$ , then

$$H(z) = \exp\left\{-\left[1 + \xi\left(\frac{z - \mu}{\sigma}\right)\right]^{-1/\xi}\right\}$$

- $\xi > 0$ : Fréchet distribution ( $G$  heavy-tailed)
- $\xi \rightarrow 0$ : Gumbel distribution ( $G$  light-tailed)
- $\xi < 0$ : Weibull distribution ( $G$  bounded upper tail)

## Pickands-Balkema-De Haan theorem

If  $G$  satisfies the FTG theorem, then the upper tail of  $G$  can be approximated by the Generalized Pareto Distribution (GPD):

$$\mathbb{P}(S \leq u + s \mid S > u) = 1 - \left(1 + \frac{\xi s}{\sigma_u}\right)^{-1/\xi}$$

for large enough  $u$ , where  $\sigma_u = \sigma + \xi(u - \mu)$ .

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So in practice, we can approximate the upper tail of many distributions by a GPD.

# Surprises and EVT

- Suppose we have  $n$  iid observations  $Y_1, \dots, Y_n$  from distribution  $F$  with density  $f$ .
- Let  $S_i = -\log f(Y_i)$  be the surprisal of  $Y_i$ .
- Then  $S_1, \dots, S_n$  are iid from the surprisal distribution  $G(s) = \mathbb{P}(S \leq s)$ .
- If  $G$  satisfies the FTG theorem, then we can approximate the upper tail of  $G$  by a GPD.

# Three-type theorem for surprises

**A1: Sub-Gaussian:**  $S = -\log f(Y)$  satisfies, for all  $\lambda \in \mathbb{R}$ , and some  $\nu > 0$ ,  $\mathbb{E} \exp\{\lambda(S - \mathbb{E}[S])\} \leq \exp\{\lambda^2 \nu^2 / 2\}$ .

**A2: Sub-exponential:**  $S$  is sub-exponential with parameters  $\nu$  and  $b$ , i.e.,  $\mathbb{E} \exp\{\lambda(S - \mathbb{E}[S])\} \leq \exp\{\lambda^2 \nu^2 / 2\}$  for all  $|\lambda| < 1/b$ .

**A3: Polynomial:**  $|S|$  has polynomial moments of order  $p \geq 1$ ; i.e.,  $\mathbb{E}[|S|^p] \leq C^p$  for some  $C > 0$  such that  $C^p - 1 > 0$ .

- A1 satisfied when  $f$  has bounded support
- A2 satisfied when  $\log f$  unbounded below, and light tails (e.g., Gaussian)
- A3 satisfied when  $f$  has heavy tails (e.g., t with df  $\geq 3$ )

# Three-type theorem for surprisals

Let  $y_1, \dots, y_n$  be an iid sequence from  $F$ ,  $S = -\log f(Y)$  where  $Y \sim F$ ,  $s_i = -\log f(y_i)$ , and  $M_n = \max\{s_1, \dots, s_n\}$ .

1 Under A1:

$$\sup_{s:s>0} \left| \mathbb{P} \left\{ |M_n - \mathbb{E}[S]| \geq \sqrt{2\nu^2 s} + \sqrt{2\nu^2 \log(2n)} \right\} - e^{-s} \right| = o(1).$$

2 Under A2:

$$\sup_{s:s>1/b} \left| \mathbb{P} \left\{ |M_n - \mathbb{E}[S]| \geq (2b)s + (2b)\log(2n) \right\} - e^{-e^{-s}} \right| = o(1).$$

3 Under A3:

$$\sup_{s:s>c} \left| \mathbb{P} \left\{ |M_n - \mathbb{E}[S]| \geq (Csn^{1/p}) \right\} - e^{-s^{-p}} \right| = o(1).$$

# Three-type theorem for surprisals

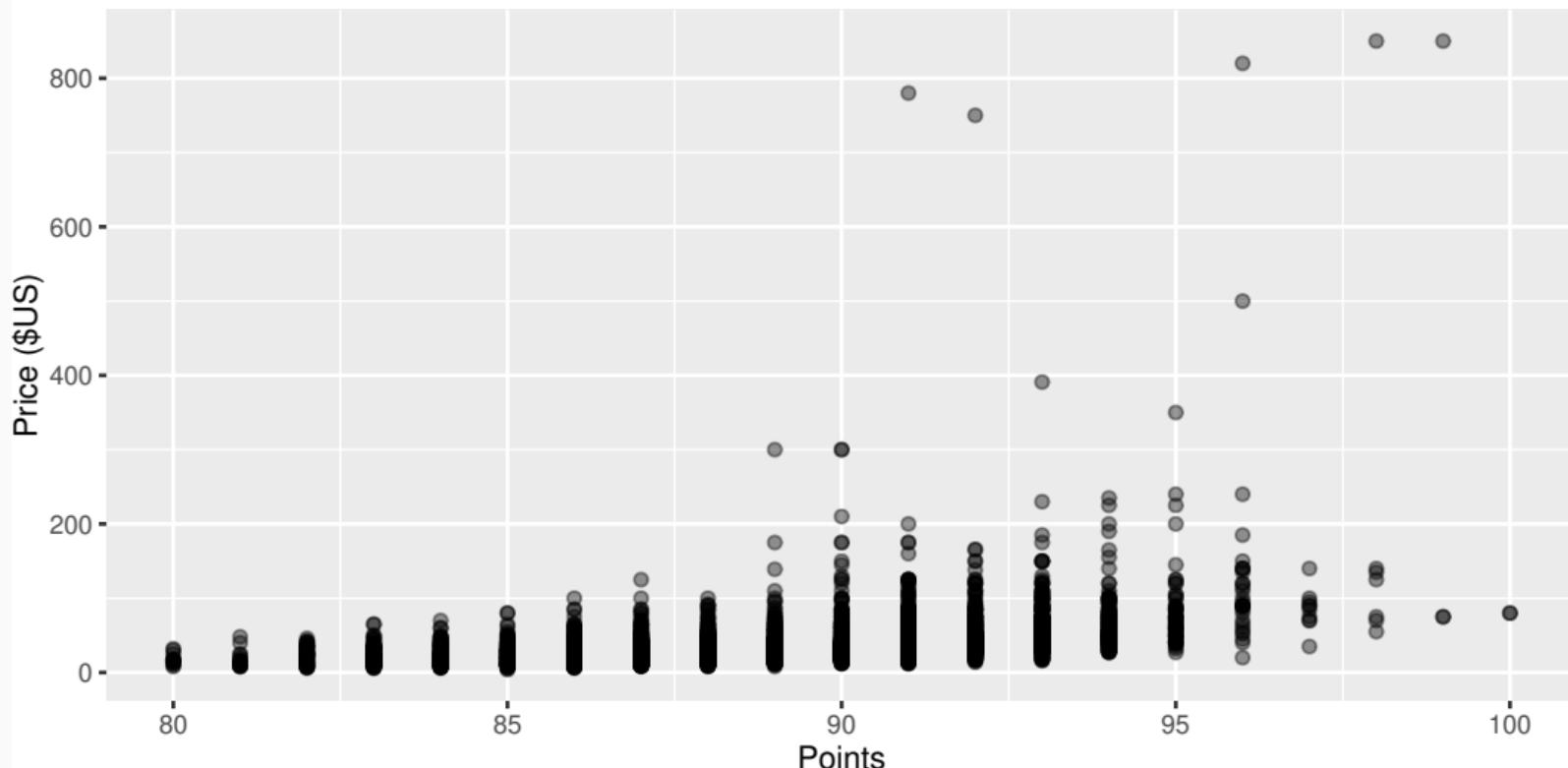
- If surprisal has Gaussian like tails, then maximum surprisal is a reversed Weibull;
- If surprisal only has an exponential moment, then maximum surprisal is Gumbel;
- If surprisal only has a polynomial moment, then maximum surprisal is Fréchet.

## Corollary

upper tail of the surprisal distribution can be approximated by a GPD, even if the assumed distribution  $F$  is incorrect, provided one of A1–A3 is satisfied.

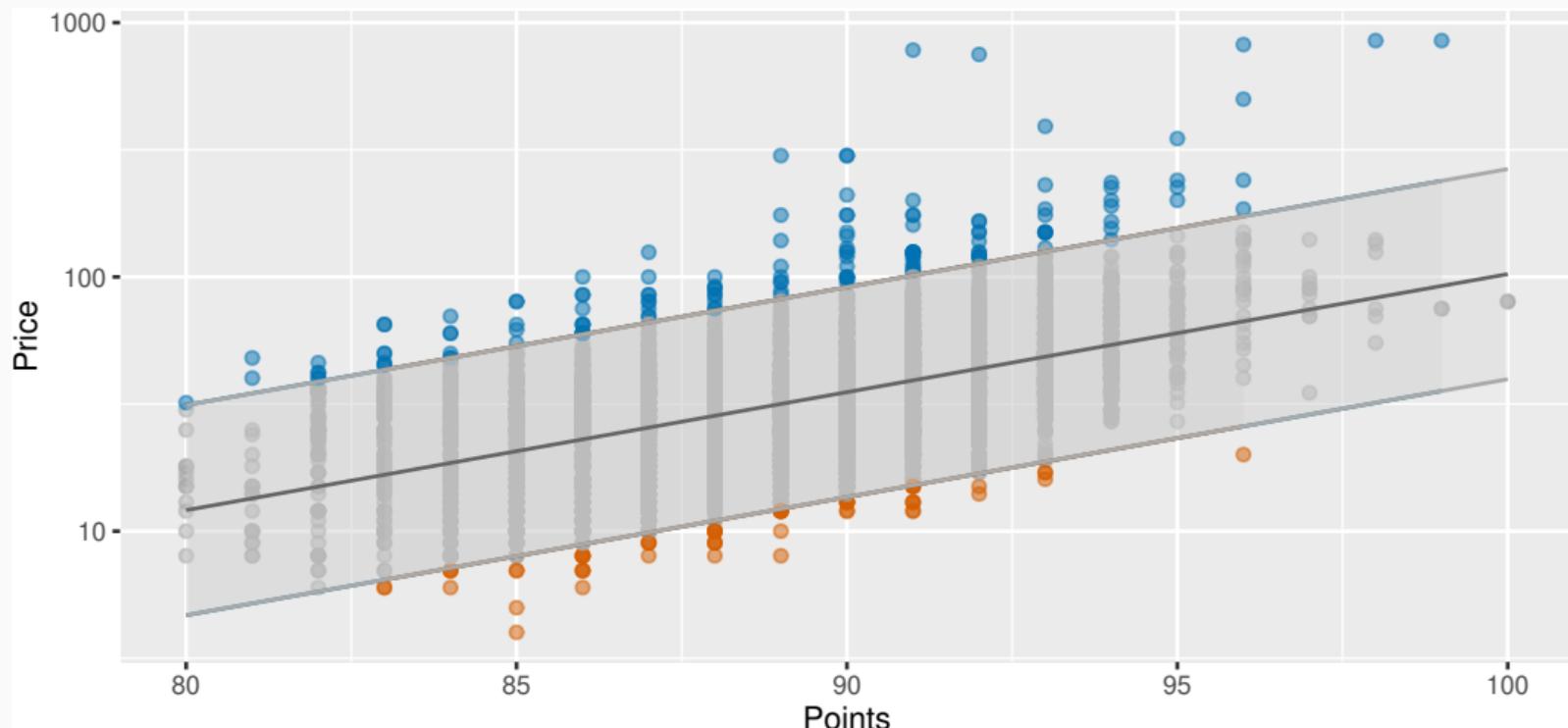
# Application to wine quality and prices

Reviews of 4496 Shiraz/Syrah wines from 'Wine Enthusiast', 15 June 2017



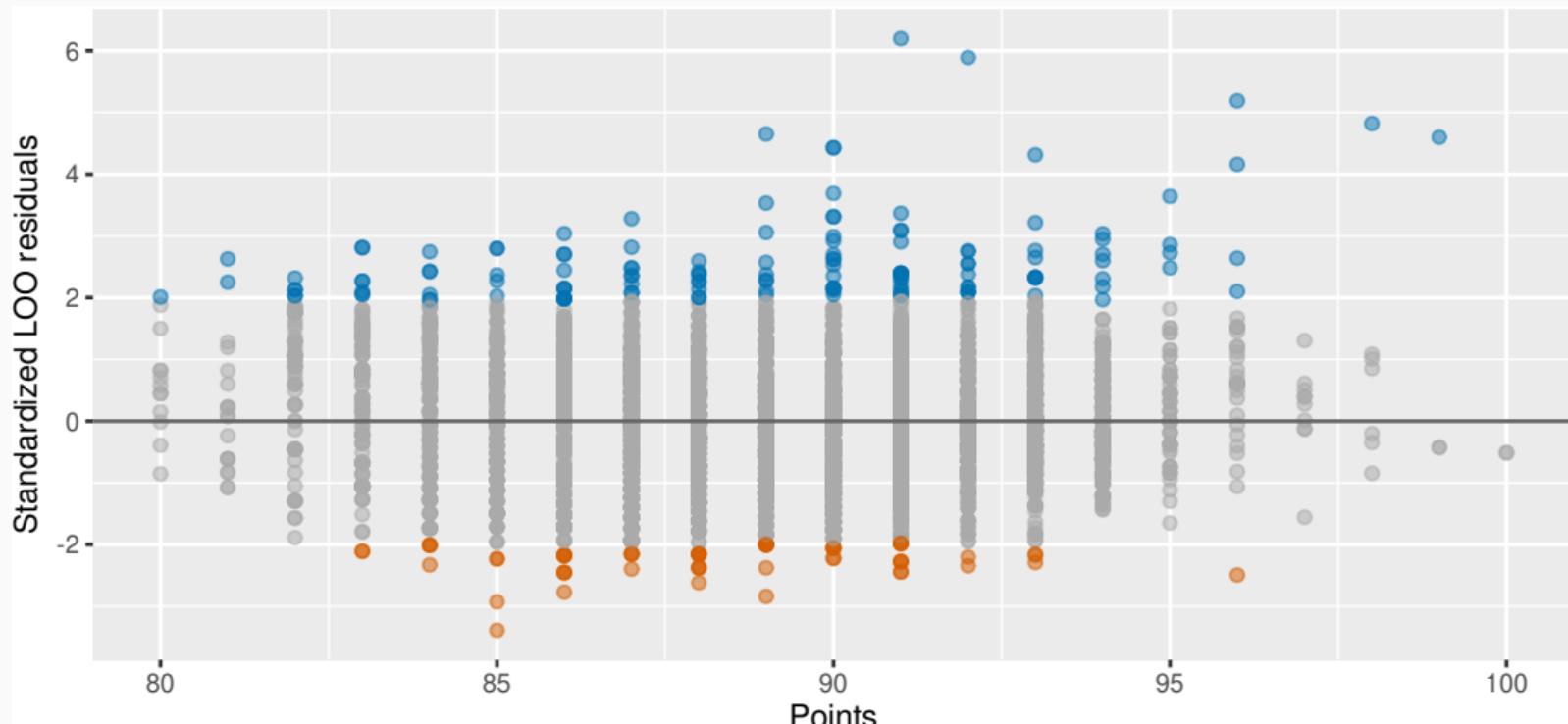
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Proposed model:  $\log \text{Price} | \text{Points} \sim N(a + b\text{Points}, \sigma^2)$ .



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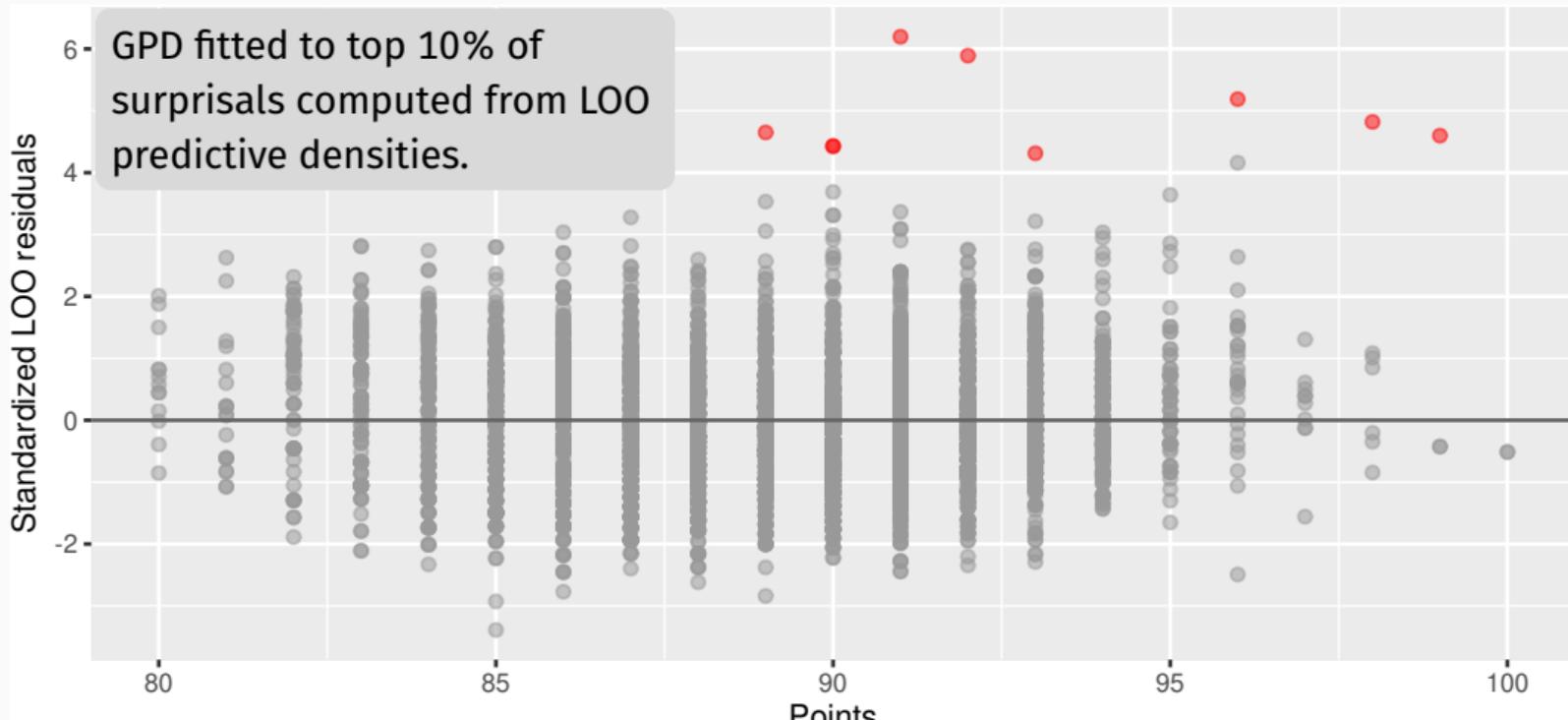
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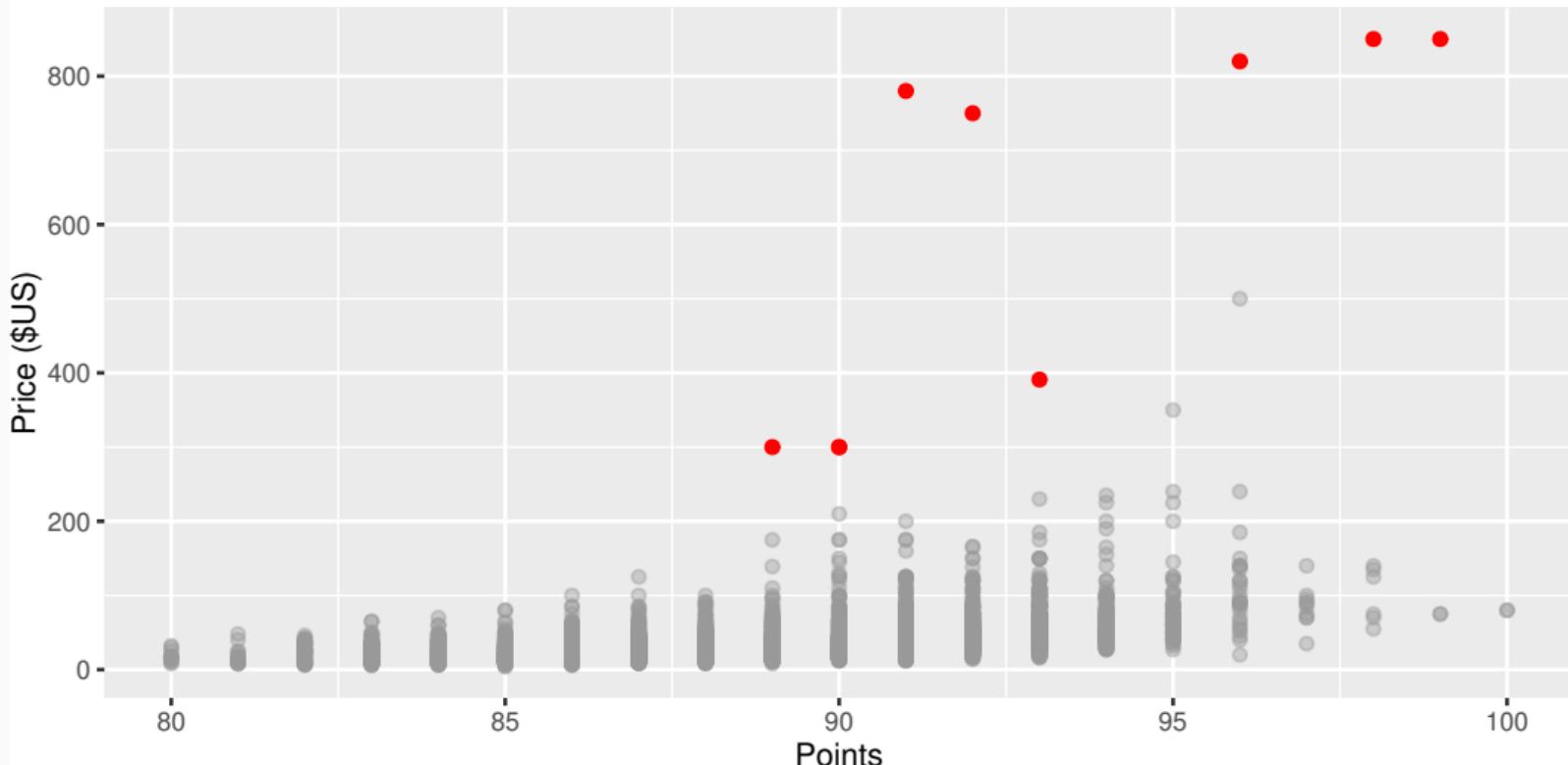
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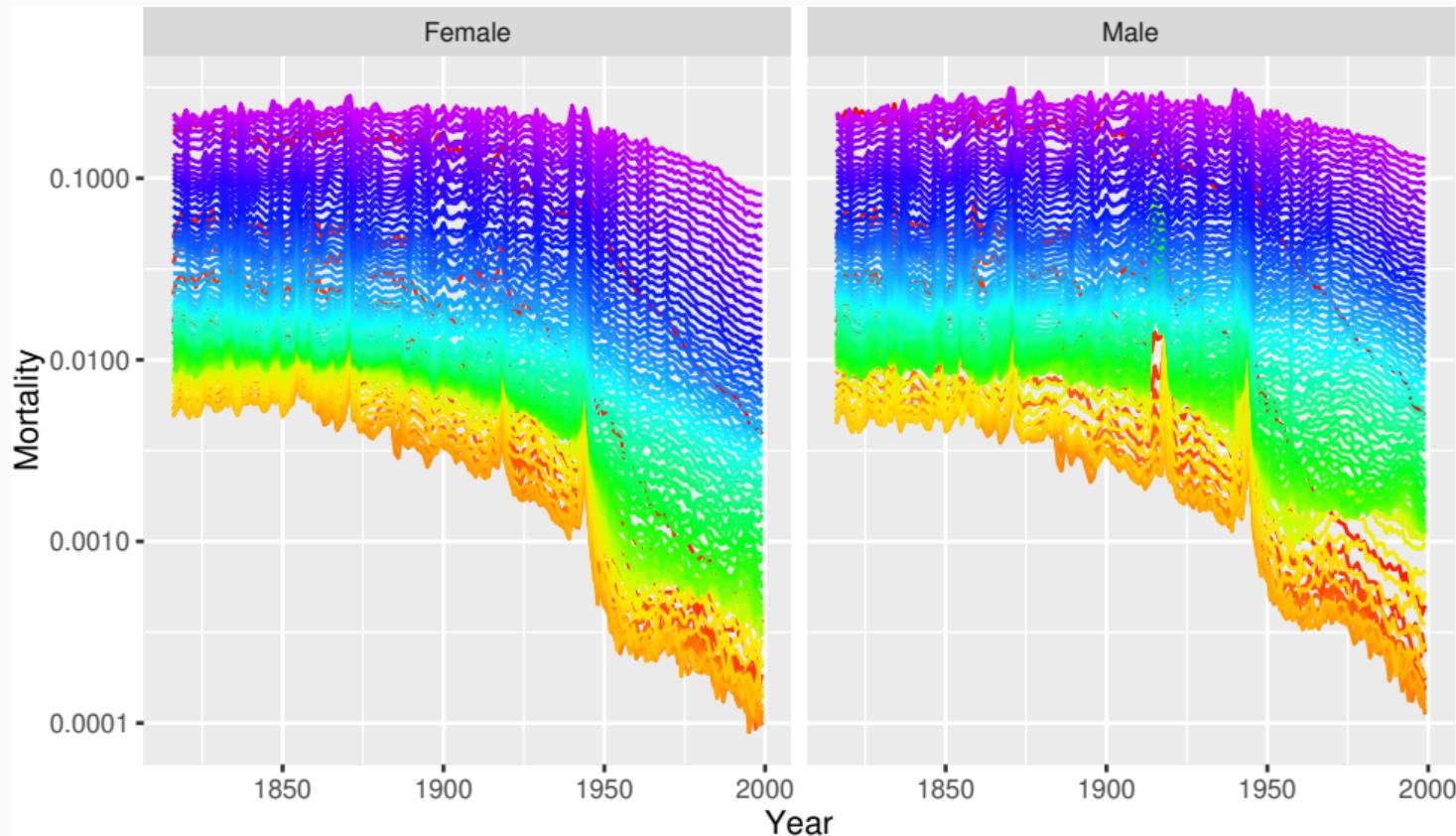


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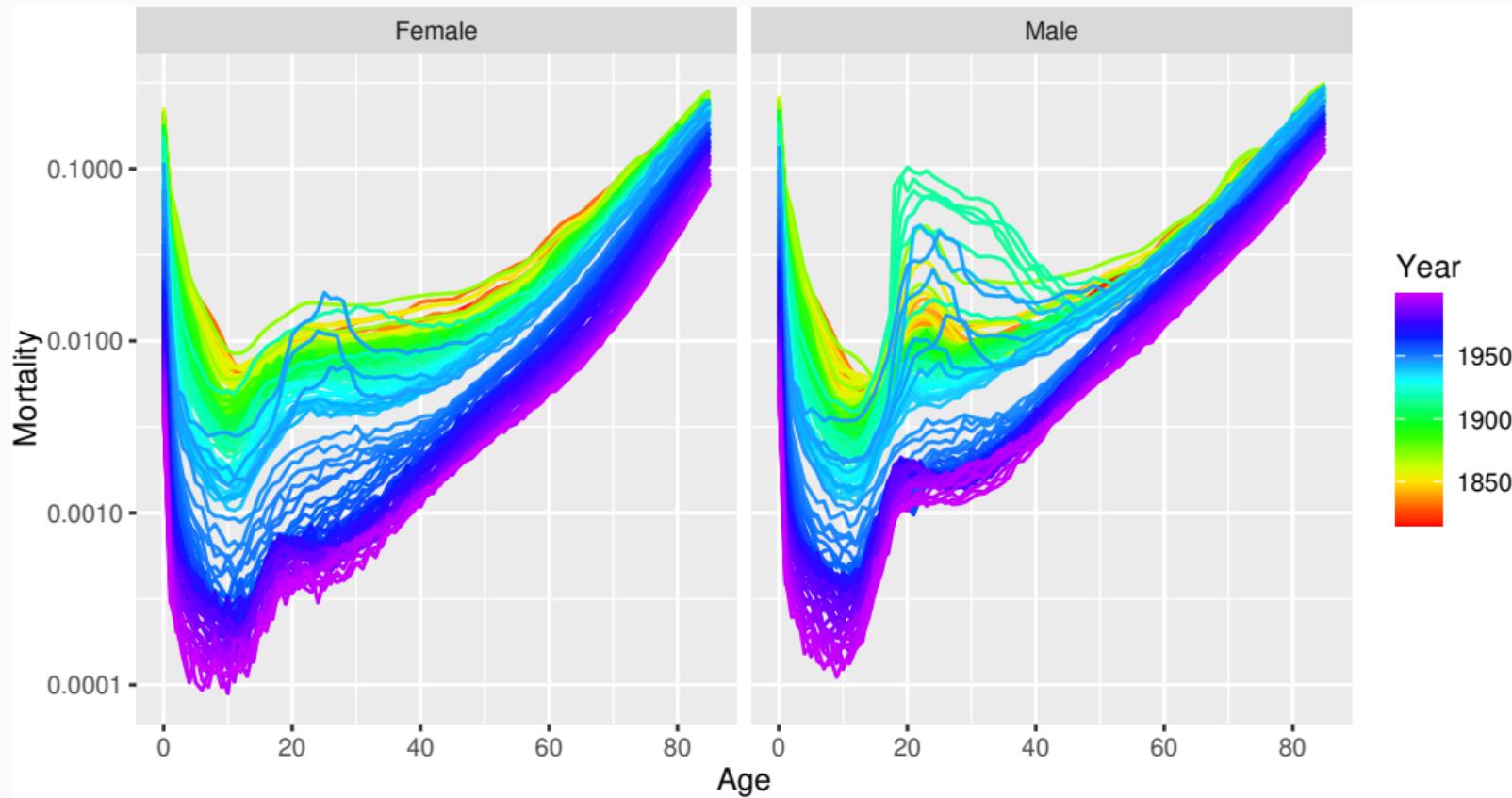
Anomalies detected ( $\alpha = 0.001$ ):

Area	Winery	Year	Points	Price
South Australia	Henschke	2009	91	780
California	Law	2013	92	750
South Australia	Henschke	2010	96	820
South Australia	Penfolds	2008	98	850
Tuscany	Tua Rita	2011	89	300
South Australia	Penfolds	2010	99	850
Tuscany	Tua Rita	2013	90	300
Tuscany	Tua Rita	2012	90	300
Rhône Valley	Domaine Jean-Michel Gerin	2013	93	391

# French mortality



# French mortality



## Application to French mortality

Model:  $\log y_t \sim N(m_t, a_t)$  where  $m_t$  and  $a_t$  are locally and robustly estimated in a window of size  $2h + 1$  around time  $t$ :

$$\hat{m}_t = \text{median}(\log y_{t-h}, \dots, \log y_{t+h})$$

$$\hat{a}_t = 1.4826 \times \text{median}(|\log y_{t-h} - \hat{m}_t|, \dots, |\log y_{t+h} - \hat{m}_t|)$$

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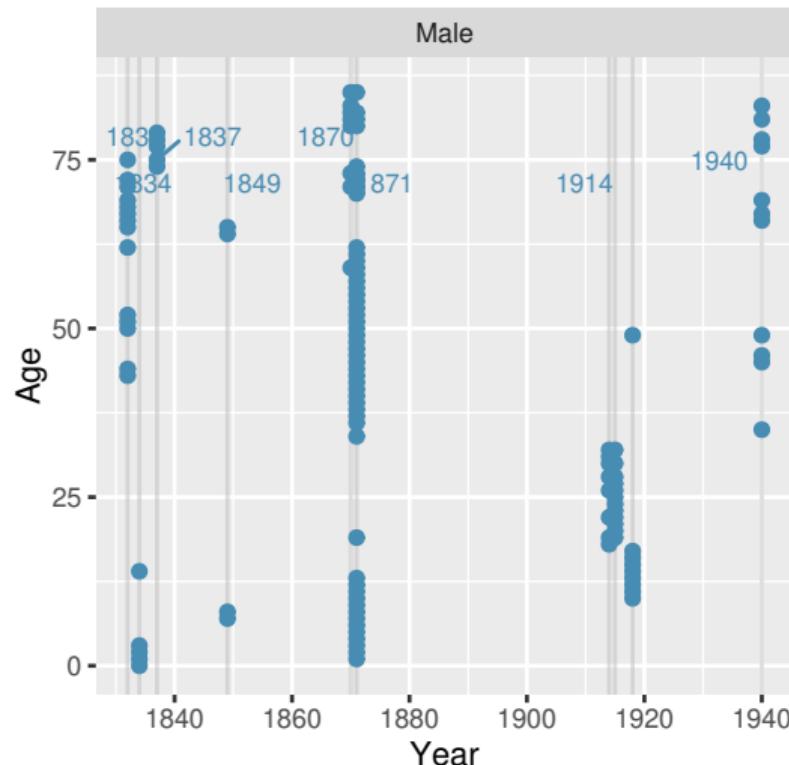
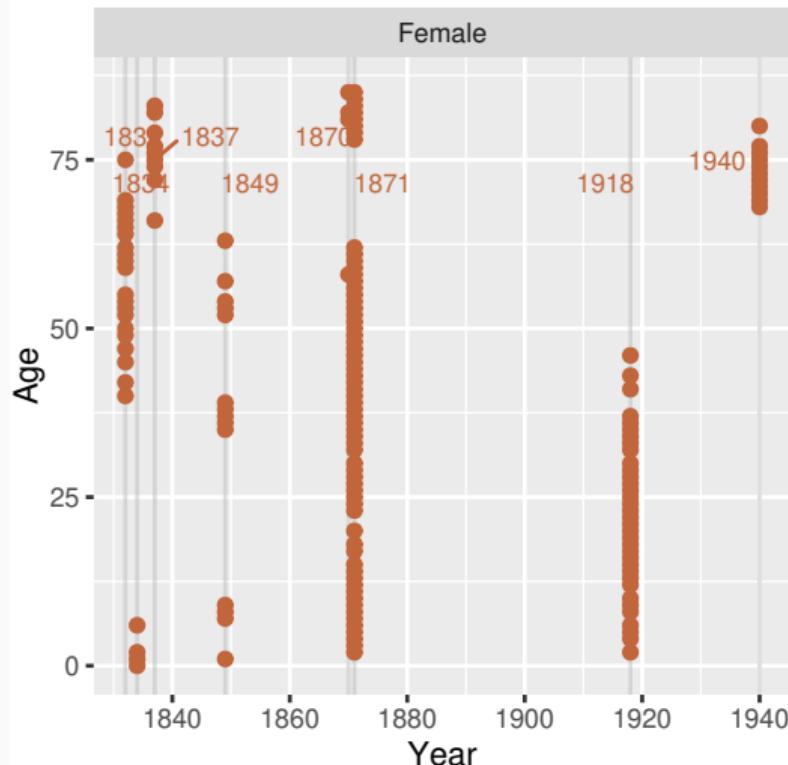
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- Male and female data from 1816–1999, over ages 0–85: 31648 observations.
- Compute surprisals under model, and surprisal probabilities under a GPD with  $\alpha = 0.01$
- Identify when at least three age groups are anomalous in same year/sex.

# Application to French mortality

French mortality anomalies



# Application to French mortality

- 1832, 1849: Cholera outbreaks
- 1870: Franco–Prussian war
- 1871: Repression of the ‘Commune de Paris’
- 1914–1918: World War I
- 1918: Spanish flu outbreak
- 1940: World War II

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# Kernel density estimation

Observations:  $\mathbf{y}_i \in \mathbb{R}^m$  for  $i \in \{1, \dots, n\}$ .

## KDE

$$\hat{f}(\mathbf{y}) = \frac{1}{n} \sum_{i=1}^n |\mathbf{H}|^{-1/2} K(\mathbf{H}^{-1/2}(\mathbf{y} - \mathbf{y}_i)),$$

- $K$  is a square-integrable spherically-symmetric function, bounded below by 0, with a finite second-order moment and unit integral.
- $\mathbf{H}$  is a symmetric  $m \times m$  positive-definite matrix.

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## LOO KDE values

$$f_{-i} = \frac{1}{n-1} (n\hat{f}(\mathbf{y}_i) - \mathbf{H}^{-1/2}K(\mathbf{0}))$$

# Kernel density estimation (consistency)

Let  $Y_1, \dots, Y_n$  be iid from square integrable density function  $f$ . Then KDE is a *consistent* estimator of  $f$  if

$$\lim_{n \rightarrow 0} E \left[ \left( \hat{f}(\mathbf{u}) - f(\mathbf{u}) \right)^2 d\mathbf{u} \right] = 0$$

For  $\hat{f}$  to be a consistent estimator,  $\mathbf{H}$  must be a symmetric positive-definite matrix that satisfies the following conditions:

- All elements of  $\mathbf{H}$  approach zero as  $n \rightarrow \infty$
- $n^{-1}|\mathbf{H}|^{-1/2} \rightarrow 0$  as  $n \rightarrow \infty$

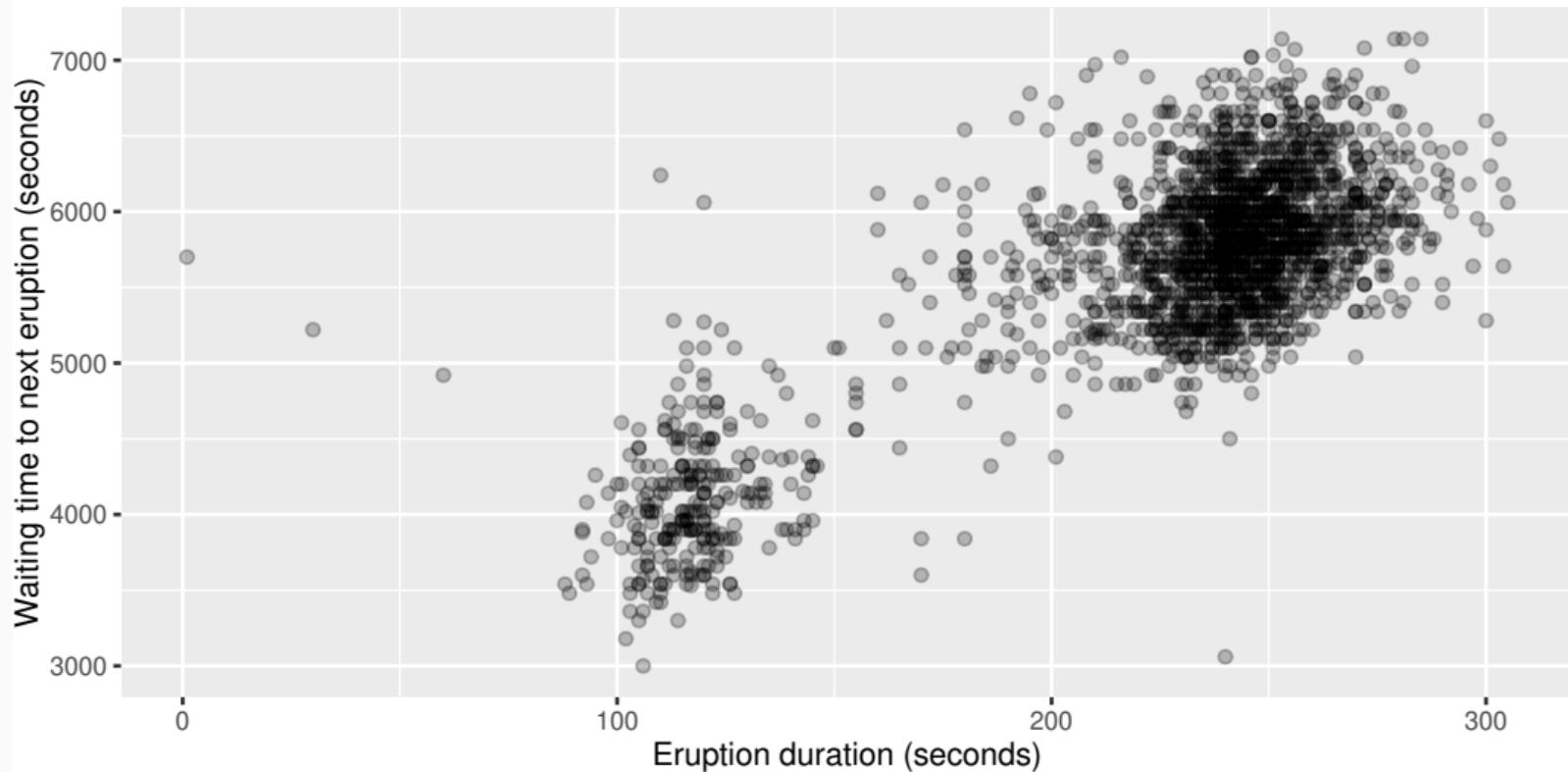
# Persistent homology

# Lookout algorithm

- 1  $\mathbf{Y}$  = data matrix with rows  $\mathbf{y}_1, \dots, \mathbf{y}_n$ .
- 2  $\hat{\Sigma}$  = orthogonalized Gnanadesikan-Kettenring estimate of  $\text{Cov}(\mathbf{Y})$ , with eigendecomposition  $\hat{\Sigma} = \mathbf{U}\mathbf{D}\mathbf{U}^\top$ .
- 3 Rotate and scale the data:  $\mathbf{Z} = \mathbf{U}\mathbf{Y}$ .
- 4 Compute persistence homology barcode of  $\mathbf{Z}$  for dim zero using Vietoris-Rips diameter; obtain ordered death diameters  $\{d_i\}_{i=1}^n$
- 5  $d^* = \gamma$  sample quantile computed from  $\{d_i\}_{i=1}^n$ .
- 6 Compute kde:  $f_i = \hat{f}(\mathbf{z}_i)$ ,  $i = 1, \dots, n$ , where  $\mathbf{H} = (d^*)^{2/m} \mathbf{I}_m$ .
- 7 Compute LOO kde values  $f_{-i} = \frac{1}{n-1} (nf_i - \mathbf{H}^{-1/2} \mathbf{K}(\mathbf{0}))$ ,  $i = 1, \dots, n$ .
- 8 Fit GPD to largest  $1 - \beta$  of surprisals  $\{-\log f_i\}_{i=1}^n$ , constraining shape parameter to be non-positive.
- 9  $p_i = (1 - \beta)P(-\log f_{-i} | \hat{\mu}, \hat{\sigma}, \hat{\xi})$ ,  $P$  = GPD cdf.

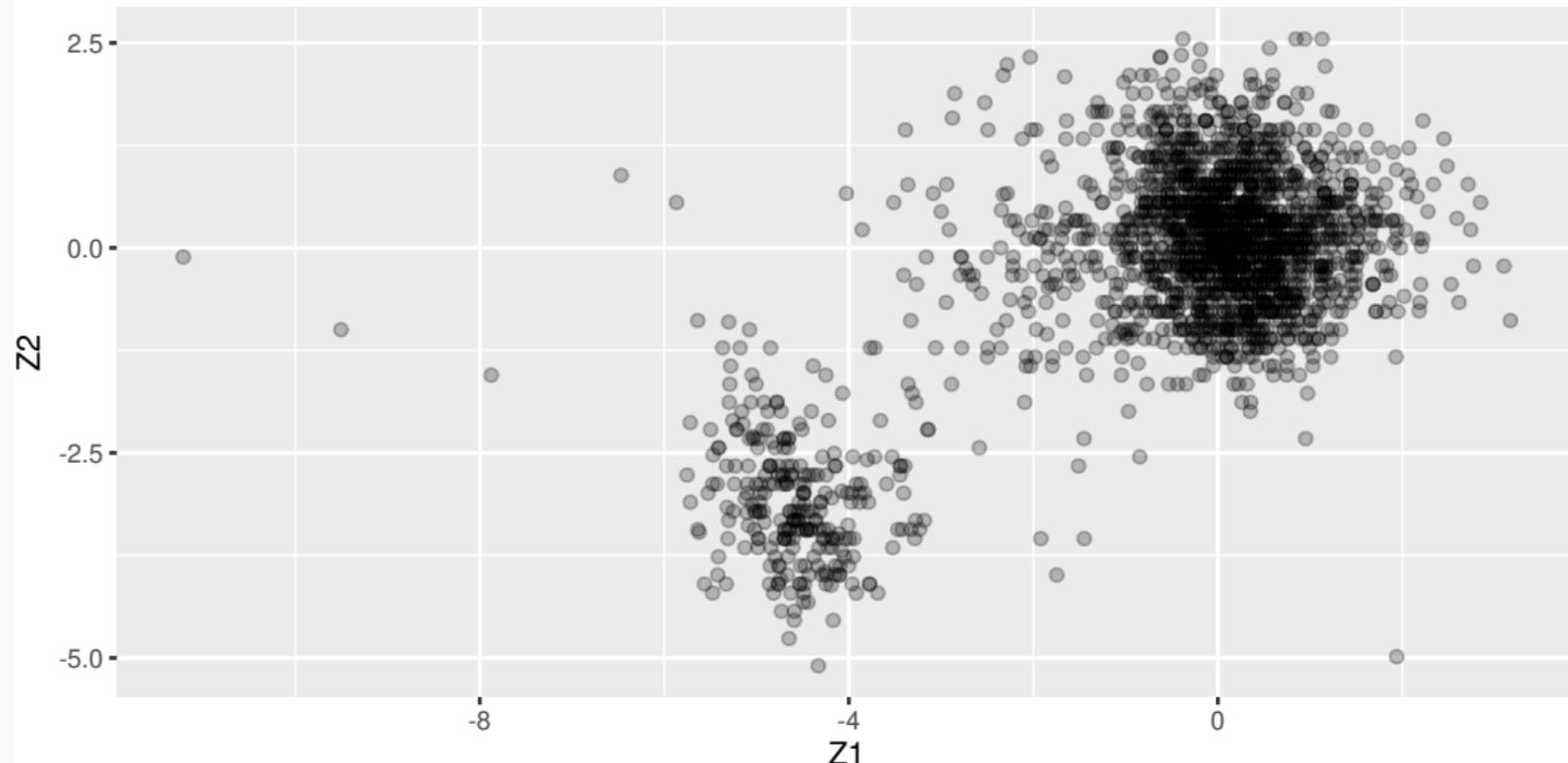
# Old Faithful eruptions

Old Faithful eruptions from 14 January 2017 to 29 December 2023



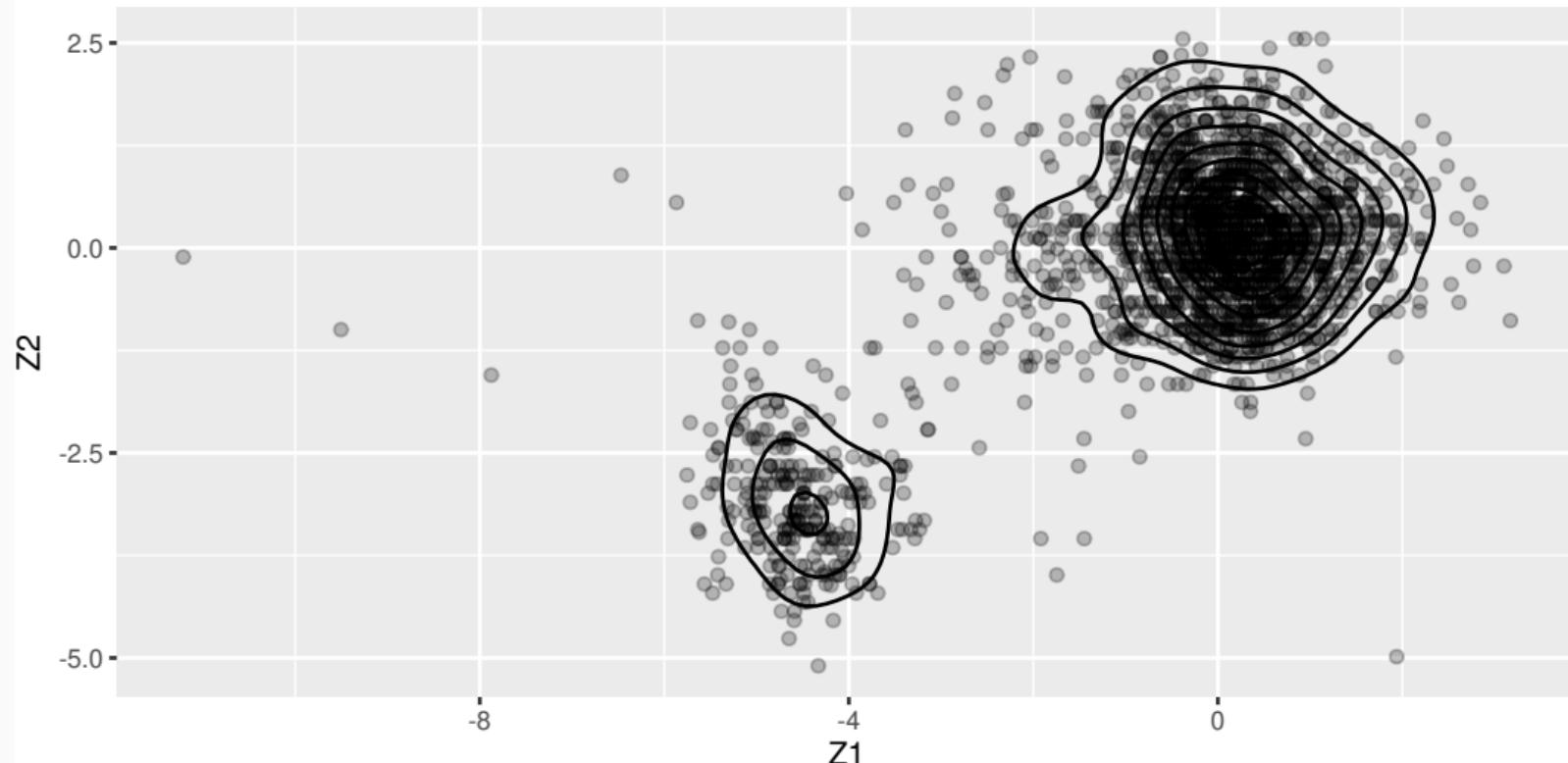
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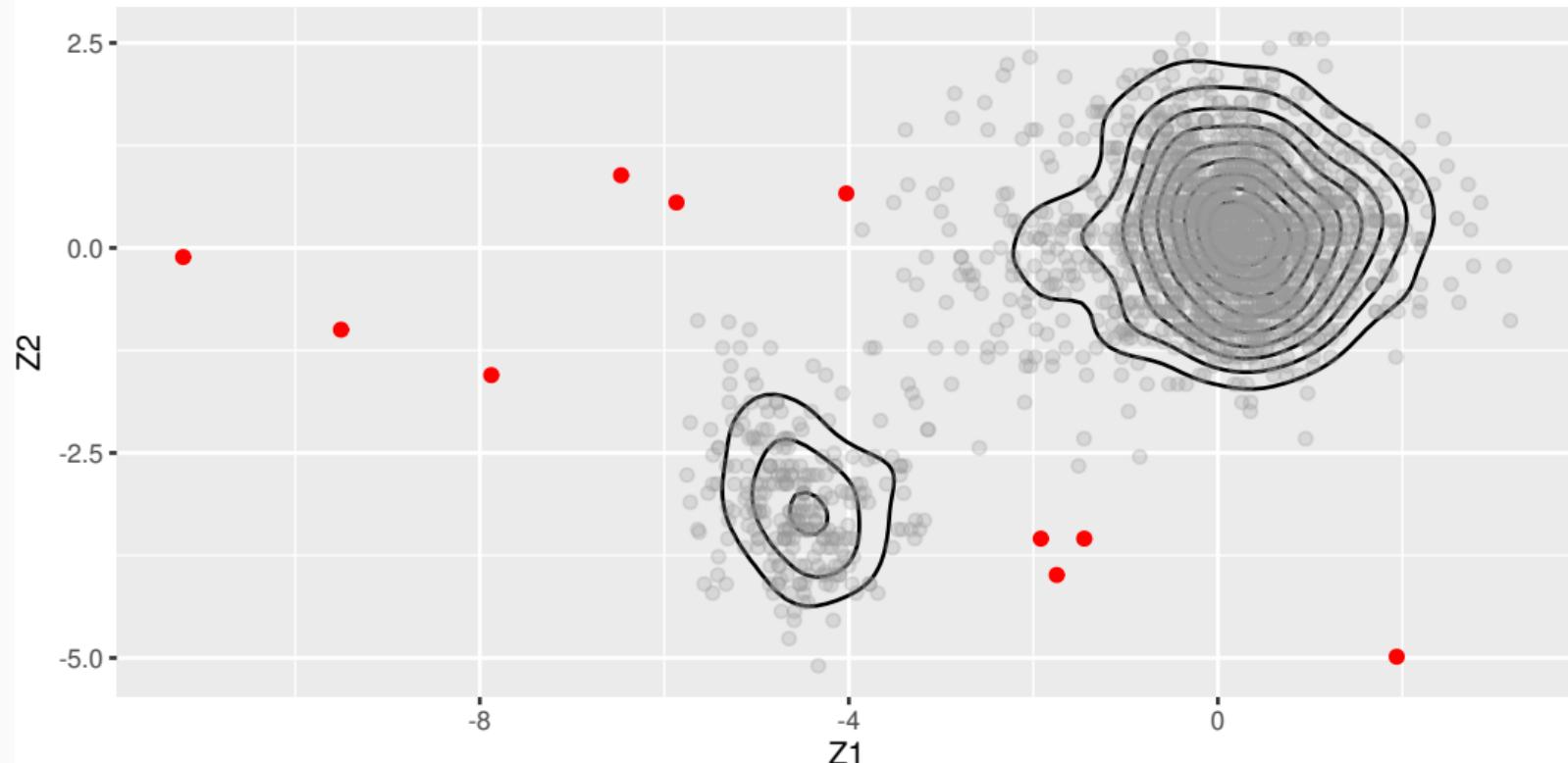
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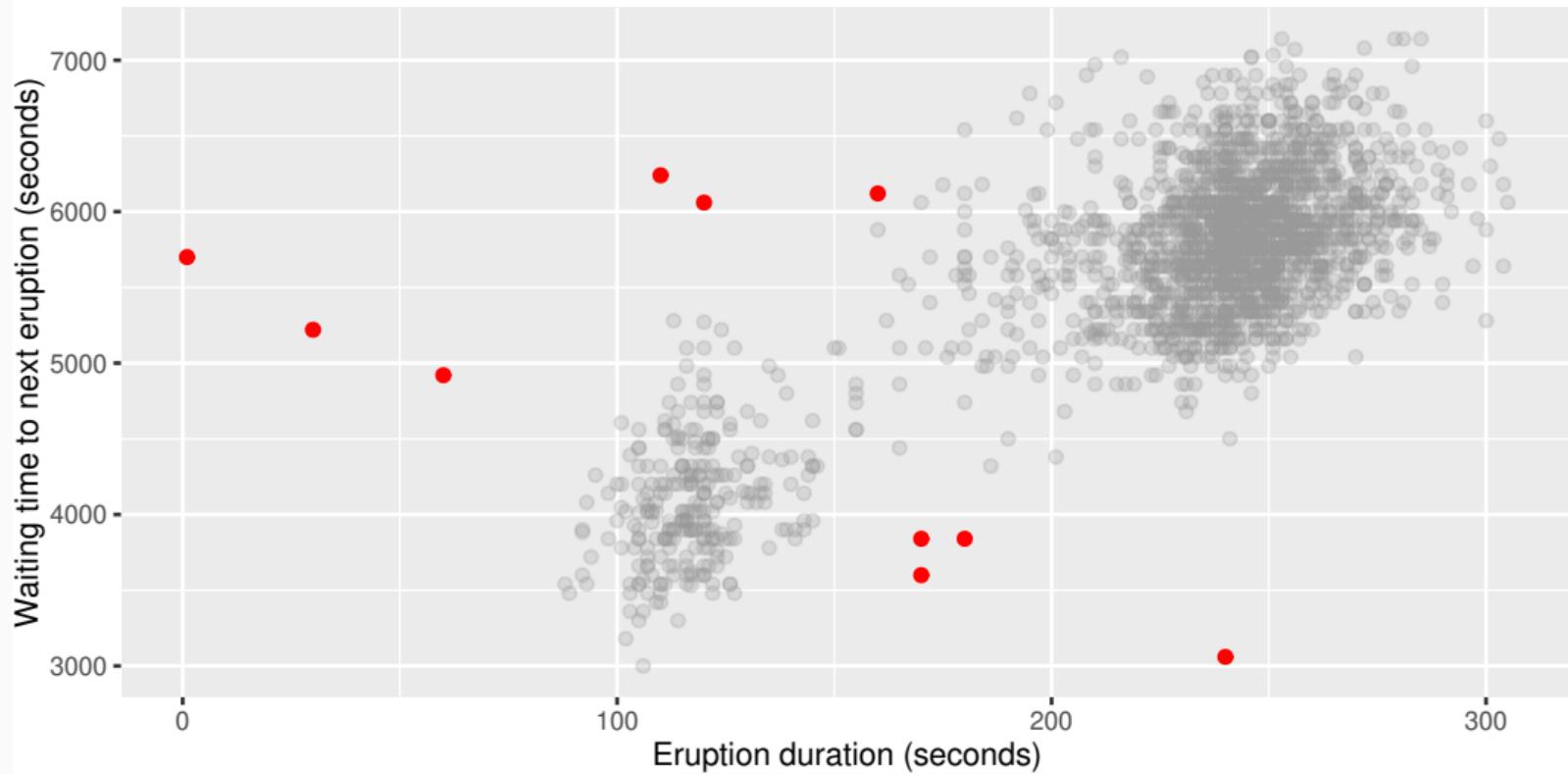
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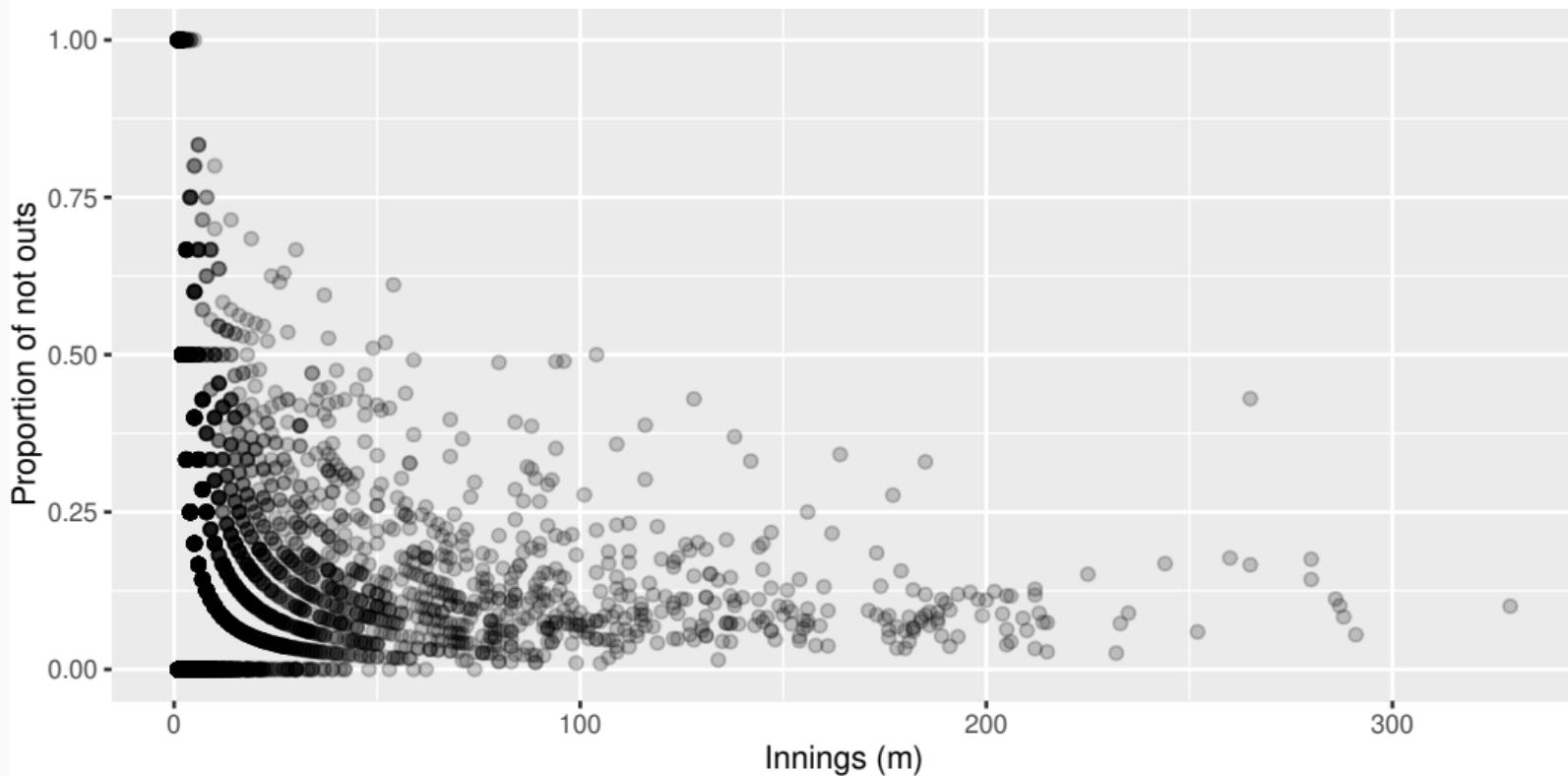
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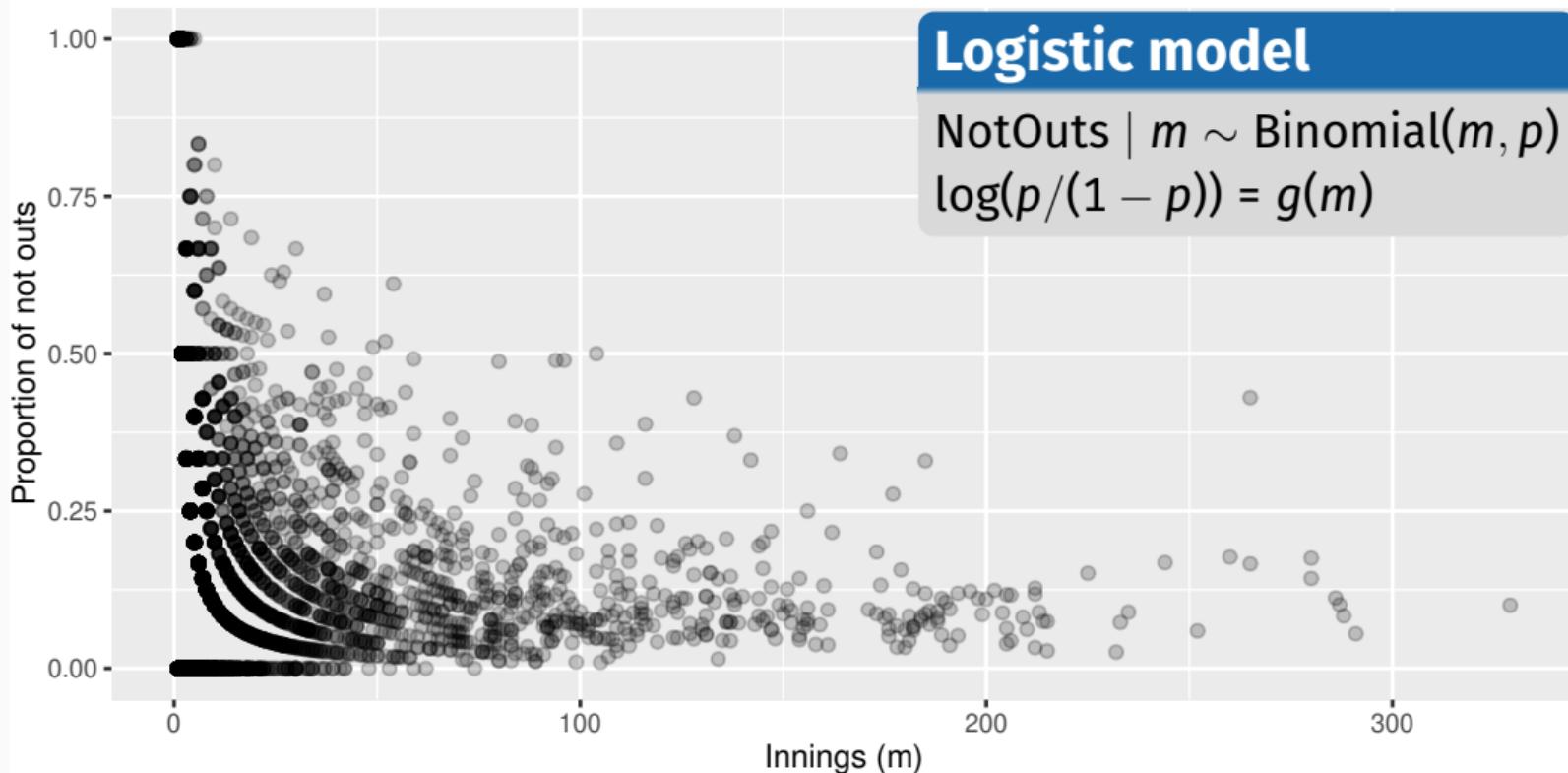
# Application to test cricket not-outs

Career batting data for all test cricketers (M+W): 1834-2025



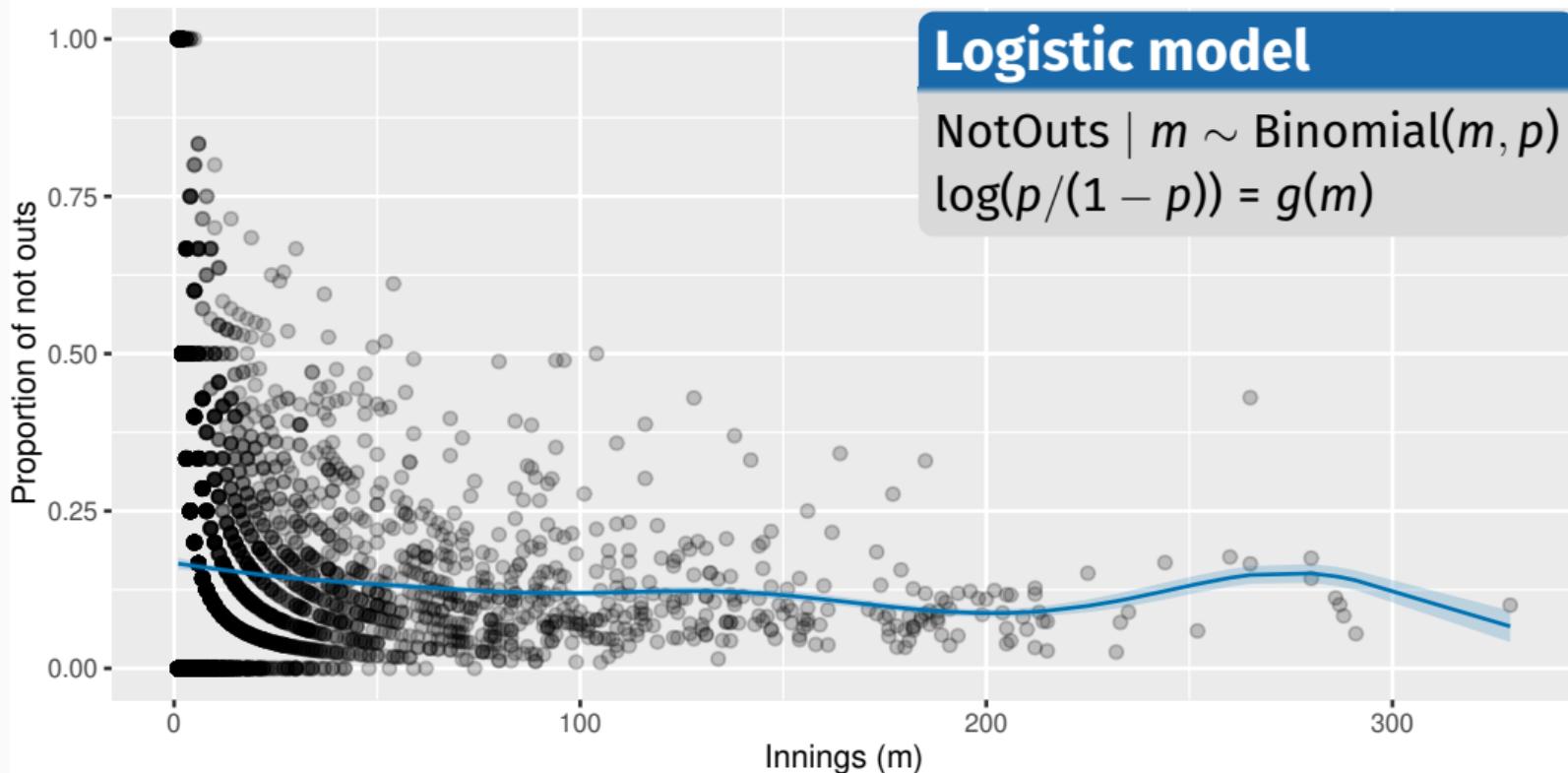
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