



Single-Fit Bootstrapping

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Single-Fit Bootstrapping



- ▶ Bootstrapping
 1. Parametric vs Non-parametric
 2. Percentile vs Studentised
 3. Many variations (e.g. conditional, stratified, balanced,...)
- ▶ All involve refitting the model (or models) many times
- ▶ Can we sometimes **avoid refitting** the model?
- ▶ Modelling zero-inflated skewed data (Fletcher et al 2005)



Single-Fit Bootstrapping



- ▶ Bootstrapping
 1. **Parametric** vs Non-parametric
 2. **Percentile** vs Studentised
 3. Many variations (e.g. conditional, **stratified**, balanced,...)
- ▶ All involve refitting the model (or models) many times
- ▶ Can we sometimes **avoid refitting** the model?
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Single-Fit Bootstrapping



Two settings of interest

1. Likelihood-based model $f_Y(Y; \beta_0)$ where
 - **n is large** enough for asymptotic likelihood theory to work
 - parameter of interest is $\theta_0 = g(\beta_0)$, with $g(\cdot)$ **non-linear**
2. Generalised linear model where
 - we have **overdispersion**
 - use quasi-likelihood (vs random effects or correlated errors)
 - want a **confidence interval** for the amount of overdispersion
 - example of a **scale parameter**



Single-Fit Bootstrapping



- ▶ Likelihood-based model $f_Y(Y; \beta_0)$ where
 - n is large enough for asymptotic likelihood theory to work
 - parameter of interest is $\theta_0 = g(\beta_0)$, with $g(\cdot)$ non-linear
- ▶ Asymptotic theory gives

$$\hat{\beta} \sim N(\beta_0, \Sigma_{\hat{\beta}})$$

where

$$\Sigma_{\hat{\beta}}^{-1} = \mathbb{E}\{-\nabla^2 \ell(\beta)\} \Big|_{\beta=\beta_0}$$

$\ell(\beta) = \text{log-likelihood}$ $\beta_0 = \text{true value of } \beta$



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- ▶ Why bootstrap?



Single-Fit Bootstrapping



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$\ell(\beta)$ = log-likelihood β_0 = true value of β

- ▶ Why bootstrap? Avoid problems with delta method...



Single-Fit Bootstrapping



- ▶ Parametric bootstrapping **pretends** that $\beta_0 = \hat{\beta}$ and uses

$$y^* \sim f_Y(Y; \hat{\beta})$$

which leads to

$$\hat{\beta}^* \sim N(\hat{\beta}, \Sigma_{\hat{\beta}^*})$$

where

$$\Sigma_{\hat{\beta}^*}^{-1} = \mathbb{E}\{-\nabla^2 \ell(\beta)\} \Big|_{\beta = \hat{\beta}}$$



Single-Fit Bootstrapping



- ▶ Parametric bootstrapping uses

$$\hat{\beta}^* \sim N(\hat{\beta}, \Sigma_{\hat{\beta}^*}) \quad \text{where} \quad \Sigma_{\hat{\beta}^*}^{-1} = \mathbb{E}\{-\nabla^2 \ell(\beta)\} |_{\beta=\hat{\beta}}$$

- ▶ But this is equivalent to

$$\hat{\beta}^* \sim N(\hat{\beta}, \hat{\Sigma}_{\hat{\beta}}) \quad \text{since} \quad \hat{\Sigma}_{\hat{\beta}}^{-1} = \mathbb{E}\{-\nabla^2 \ell(\beta)\} |_{\beta=\hat{\beta}}$$



Single-Fit Bootstrapping



- ▶ Parametric bootstrapping equivalent to using

$$\hat{\beta}^* \sim N(\hat{\beta}, \hat{\Sigma}_{\hat{\beta}}) \quad \hat{\theta}^* = g(\hat{\beta}^*)$$

- ▶ Requires **no refitting** of the model
- ▶ **Percentiles** of $\hat{\theta}^*$ provide a confidence interval



Single-Fit Bootstrapping



- ▶ Parametric bootstrapping equivalent to using

$$\hat{\beta}^* \sim N(\hat{\beta}, \hat{\Sigma}_{\hat{\beta}}) \quad \hat{\theta}^* = g(\hat{\beta}^*)$$

- ▶ Requires **no refitting** of the model
- ▶ **Percentiles** of $\hat{\theta}^*$ provide a confidence interval
- ▶ c.f. asymptotic Bayes
 - $p(\beta|y) \approx N(\hat{\beta}, \hat{\Sigma}_{\hat{\beta}})$
 - Posterior distribution vs Bootstrap distribution
 - Hastie, Tibshirani and Friedman (2009)



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Example 1: Zero-inflated count data

- ▶ Hurdle (or mixture) model
 1. Binomial model for probability of a zero
 2. (Zero-truncated) negative binomial model for non-zeros
- ▶ $\mathbb{E}(Y) = \text{non-linear}$ function of the two sets of β 's

Example 2: Probability of surviving to adulthood

- ▶ Mark-recapture model (e.g. chicks banded at fledging)

$$S_{0A} = S_J^k \quad (k = \text{age at reaching adulthood})$$

$$\log\left(\frac{S_J}{1-S_J}\right) = \beta_0 + \beta_1 x_1 + \dots$$

Example 3: Tim's maxima...

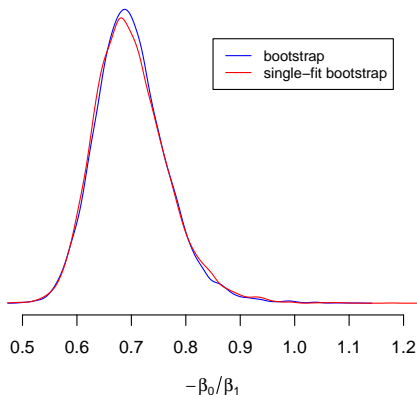


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Example 4: LD50

- ▶ Binomial model: $\log\left(\frac{\pi}{1-\pi}\right) = \beta_0 + \beta_1 x$ (LD50 = $-\beta_0/\beta_1$)
- ▶ Example: $n = 30$, $m = 10$, $\beta_0 = -1$, $\beta_1 = 1.6$, $x \in [0, 1]$



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Confidence Interval for Overdispersion (with Michel de Lange)

► Overdispersion

- Arises when fitting a generalised linear model to count data
- Greater variation in Y than we would expect from the model
- Occurs with binomial, Poisson and multinomial models
- Leads to
 1. Confidence intervals being **too narrow**
 2. Model selection/averaging: **too much weight** to larger models

► Motivation: mark-recapture data (**multinomial** models)

- Multi-state mark-recapture models can take a while to fit
- Standard bootstrapping not straightforward to apply



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- ▶ Reasons for overdispersion
 1. **Heterogeneity** in model parameters (e.g. probability of survival)
 2. **Dependence** in observations (e.g. breeding pair of birds)

- ▶ Possible remedies
 1. Add a **random effect** (e.g. individual probabilities of survival)
 2. Model the **dependence** structure (less common, more difficult)

- ▶ Semi-parametric approach: Quasi-likelihood
 1. Robust to model-misspecification
 - special case of **robust likelihood** (Royall and Tsou 2003)
 2. Simple to use (**adjust** intervals, model selection/averaging)



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Quasi-likelihood

- ▶ Specify only the mean and variance of Y
- ▶ $\text{var}(Y_i) = \phi V_i$ ($i = 1, \dots, n$)
- ▶ V_i = variance of Y predicted by the **assumed** model
- ▶ Estimate of ϕ used to adjust
 1. Confidence intervals (**wider**)
 2. Model selection/averaging (**less weight** to larger models)



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- ▶ Mark-recapture setting (**multinomial** models)
 1. Farzana Afroz PhD: better point estimator of ϕ
 2. How reliable is the estimator?
- ▶ Confidence interval for ϕ
 1. Useful in its own right (**this talk**)

e.g. $\hat{\phi} = 4.6$; CI = [0.8, 10.3] vs [4.1, 5.4]
 2. Effect on (**future work**)
 - ▶ Confidence intervals for model parameters
 - ▶ Model selection/averaging



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- ▶ Confidence interval for ϕ using the **pivot**

$$(n - p)\hat{\phi}/\phi \sim \chi_{n-p}^2$$

- ▶ Leads to a $100(1 - 2\alpha)\%$ interval given by

$$(n - p)\hat{\phi}/\phi_L = \chi_{n-p, 1-\alpha}^2 \quad (n - p)\hat{\phi}/\phi_U = \chi_{n-p, \alpha}^2$$

- ▶ What if $(n - p)\hat{\phi}/\phi$ **not** χ_{n-p}^2 ?

(e.g. $\phi > 1$ and/or n small)



Single-Fit Bootstrapping



- ▶ Confidence interval for ϕ using the **approximate pivot**

$$(n - p)\hat{\phi}/\phi \sim G_{n-p}$$

- ▶ Use bootstrap to estimate G_{n-p} (c.f. **studentised** bootstrap)

1. B bootstrap estimates give $(n - p)\hat{\phi}_b^*/\hat{\phi}$ ($b = 1, \dots, B$)
2. Relevant percentiles of bootstrap distribution give

$$\phi_L = \hat{\phi}^2/\hat{\phi}_{1-\alpha}^* \quad \phi_U = \hat{\phi}^2/\hat{\phi}_{\alpha}^*$$

- ▶ Resample Y and **refit** the model OR **resample the residuals?**

$$\hat{\phi}_1 = \sum_{i=1}^n e_i^2/(n - p) \quad \text{where} \quad e_i = (y_i - \hat{\mu}_i)/\hat{V}_i^{1/2}$$

$$\hat{\phi}_2 = \hat{\phi}_1/(1 + \bar{s}) \quad \text{where} \quad s_i = (y_i - \hat{\mu}_i)/\hat{V}_i$$



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- ▶ Resampling the residuals

$$\hat{\phi}_1 = \sum_{i=1}^n e_i^2 / (n - p) \quad \text{where} \quad e_i = (y_i - \hat{\mu}_i) / \hat{V}_i^{1/2}$$

$$\hat{\phi}_2 = \hat{\phi}_1 / (1 + \bar{s}) \quad \text{where} \quad s_i = (y_i - \hat{\mu}_i) / \hat{V}_i$$

- ▶ $\hat{\phi}_2$ has smaller variance (especially when data are sparse)
- ▶ “hat-values” allowed for in the denominator ($n - p$)
- ▶ Avoids the need for **conditioning** upon $\hat{\mu}_i$ (McCullagh 1986)



Single-Fit Bootstrapping



- ▶ Resampling the residuals

$$\hat{\phi}_1 = \sum_{i=1}^n e_i^2 / (n - p) \quad \text{where} \quad e_i = (y_i - \hat{\mu}_i) / \hat{V}_i^{1/2}$$

$$\hat{\phi}_2 = \hat{\phi}_1 / (1 + \bar{s}) \quad \text{where} \quad s_i = (y_i - \hat{\mu}_i) / \hat{V}_i$$

- ▶ $\mathbb{E}(e_i) \approx 0$ $\mathbb{E}(e_i^2) \approx \left(\frac{n-p}{n}\right)\phi$ $\mathbb{E}(e_i e_j) \approx 0$

e_i **approximately** exchangeable up to **second** moment

- ▶ $\mathbb{E}(e_i^3) \propto V_i' / V_i^{1/2} \implies$ **not** exchangeable on 3rd moment

Stratify by $V_i' / V_i^{1/2}$ (Davison and Hinkley, 1997)



Single-Fit Bootstrapping



- ▶ Resampling the residuals

$$\hat{\phi}_1 = \sum_{i=1}^n e_i^2 / (n - p) \quad \text{where} \quad e_i = (y_i - \hat{\mu}_i) / \hat{V}_i^{1/2}$$

$$\hat{\phi}_2 = \hat{\phi}_1 / (1 + \bar{s}) \quad \text{where} \quad s_i = (y_i - \hat{\mu}_i) / \hat{V}_i$$

- ▶ $\mathbb{E}(s_i) \approx 0$ $\mathbb{E}(s_i^2) \approx \left(\frac{n-p}{n}\right)\phi/V_i$ $\mathbb{E}(s_i s_j) \approx 0$

s_i **approximately** exchangeable on **first** moment only

$\hat{\phi}_2$ better for point estimation

what about interval estimation?



Single-Fit Bootstrapping



- ▶ Resampling the residuals

$$\hat{\phi}_1 = \sum_{i=1}^n e_i^2 / (n - p) \quad \text{where} \quad e_i = (y_i - \hat{\mu}_i) / \hat{V}_i^{1/2}$$

$$\hat{\phi}_2 = \hat{\phi}_1 / (1 + \bar{s}) \quad \text{where} \quad s_i = (y_i - \hat{\mu}_i) / \hat{V}_i$$

- ▶ $\mathbb{E}(e_i) \approx 0$ $\mathbb{E}(e_i^2) \approx \frac{n-p}{n} \phi$ $\mathbb{E}(e_i e_j) \approx 0$

- ▶ Set $u_i = \frac{n}{n-p} e_i^2$

Estimate $\mathbb{E}(U_i) \approx \phi$ by $\hat{\phi}_1 = \frac{1}{n} \sum_{i=1}^n u_i$ (sample mean)

Resampling the “observations” u_i



Single-Fit Bootstrapping



- ▶ Resampling the **residuals**

$$\hat{\phi}_1^* = \sum_{i=1}^n e_i^{*2} / (n - p)$$

$$\hat{\phi}_2^* = \hat{\phi}_1^* / (1 + \bar{s})$$

e_i^* randomly sampled from the e_i ($i = 1, \dots, n$)

- ▶ **No refitting** of the model required
- ▶ What about the s_i ?

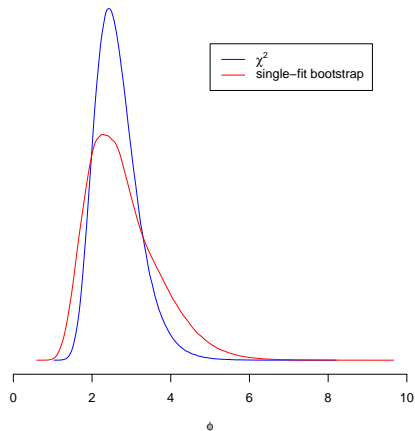
Use of $s_i^* = e_i^* / \hat{V}_i^{1/2}$ can lead to $\hat{\phi}_2^* < 0$



Single-Fit Bootstrapping



- ▶ Flamingo data (615 adults; 1982–1987; Camargue, France)
- ▶ Confidence distributions for ϕ based on $\hat{\phi}_2$



Single-Fit Bootstrapping



Simulations from mark-recapture model

- ▶ $\text{var}(Y_{ij}) = \phi\mu_{ij}$ (release-cohort i , capture-history j)
- ▶ 6-year study, 100 newly-ringed individuals released each year
- ▶ $\phi = 2.5$, $S = 0.95$, $P = 0.75$
- ▶ Results for 90% interval using $\hat{\phi}_2$

	Coverage	Median Width
χ^2	0.84	1.65
Single-fit bootstrap	0.87	1.83



Single-Fit Bootstrapping



Simulations from mark-recapture model

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- ▶ 6-year study, 10 newly-ringed individuals released each year
- ▶ $\phi = 2.5$, $S = 0.95$, $P = 0.75$
- ▶ Results for 90% interval using $\hat{\phi}_2$

	Coverage	Median Width
χ^2	0.50	1.25
Single-fit bootstrap	0.88	2.63



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Simulations from negative binomial model

- ▶ $\text{var}(Y_i) = \phi\mu_i$ $\log(\mu_i) = \beta_0 + \beta_1 x_{1i}$
- ▶ $n = 30$, $\phi = 2 - 5$, $\beta_0 = -2$, $\beta_1 = 4$ ($0.1 < \mu_i < 8$)
- ▶ Coverage for 90% interval using $\hat{\phi}_2$

	ϕ			
	2	3	4	5
χ^2	0.79	0.70	0.61	0.61
Single-fit bootstrap	0.89	0.87	0.84	0.84



Single-Fit Bootstrapping



- ▶ Two settings where **single-fit** bootstrapping is useful
 1. Likelihood-based model with large n and $\theta = g(\beta)$ **non-linear**
 2. Estimation of a **scale** parameter (e.g. overdispersion in GLMs)
- ▶ θ involves location **and** scale parameters? (Fletcher et al 2005)
- ▶ Already used in practice? (e.g. Brooks and Morgan 2000)
- ▶ Other settings?





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