

# The Bootstrap Method

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# Motivation

► **Normal Regression Model:**  $y_i = \mathbf{x}'_i \boldsymbol{\beta} + \varepsilon_i$ ,  $\varepsilon_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ .

► *MLE:*  $\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$

► *Confidence Intervals:*  $\hat{\boldsymbol{\beta}} \sim \mathcal{N}(\boldsymbol{\beta}, \sigma^2 \mathbf{V})$ ,  $\mathbf{V} = (\mathbf{X}'\mathbf{X})^{-1}$ .

⇒ 95% CI for  $\beta_j$  is  $\hat{\beta}_j \pm 1.96 \cdot \hat{\sigma} V_{jj}^{1/2}$ , where  $\hat{\sigma}$  is the MLE of  $\sigma$ .

(This is the Observed Fisher Information method, which is indistinguishable from the exact CI based on the  $t_{(n-p)}$  distribution for  $n - p > 30$ .)

# Motivation

- ▶ **Normal Regression Model:**  $y_i = \mathbf{x}'_i \boldsymbol{\beta} + \varepsilon_i$ ,  $\varepsilon_i \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ .
- ▶ **Relaxed Assumptions:**  $y_i = \mathbf{x}'_i \boldsymbol{\beta} + \varepsilon_i$ ,  $\varepsilon_i \stackrel{\text{iid}}{\sim} f(\varepsilon)$ ,  
 $E[\varepsilon_i] = 0$ ,  $\text{var}(\varepsilon_i) = 1$ .
- ▶ *Estimator:* Under Relaxed Assumptions,  $\hat{\boldsymbol{\beta}}$  is the **Best Linear Unbiased Estimator** (BLUE), in the sense that for any  $\tilde{\boldsymbol{\beta}} = \mathbf{A}\mathbf{y}$  with  $E[\tilde{\boldsymbol{\beta}}] = \boldsymbol{\beta}$ ,

$$\text{var}(\mathbf{a}'\hat{\boldsymbol{\beta}}) \leq \text{var}(\mathbf{a}'\tilde{\boldsymbol{\beta}}), \quad \mathbf{a} \in \mathbb{R}^p.$$

- ▶ *Confidence Intervals:* By linearity still have  $\text{var}(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$ . Turns out that normality-based CI is asymptotically valid.

# Motivation

- ▶ **Mean Regression:**  $E[y | \mathbf{x}] = \mathbf{x}'\beta$ .
- ▶ **Quantile Regression:** Define the  $\tau$ -level **quantile function**

$$q_\tau(y | \mathbf{x}) = F_{y|\mathbf{x}}^{-1}(\tau | \mathbf{x}) \quad \iff \quad \Pr\{y \leq q_\tau(y | \mathbf{x}) | \mathbf{x}\} = \tau.$$

The QR model is

$$q_\tau(y | \mathbf{x}) = \mathbf{x}'\beta_\tau,$$

for any  $\mathbf{x} \in \mathbb{R}^p$  and specific  $\tau \in (0, 1)$  (or multiple  $\tau$  each with their own  $\beta_\tau$ ).

# Quantile Regression

## Examples

1. **Additive Model:**  $y = \mathbf{x}'\boldsymbol{\beta} + \varepsilon$ , where  $\varepsilon$  is an arbitrary error independent of  $\mathbf{x}$ .

$$\implies q_{\tau}(y \mid \mathbf{x}) = \mathbf{x}'\boldsymbol{\beta} + q_{\tau}(\varepsilon).$$

# Quantile Regression

## Examples

**2. Location-Scale Model:**  $y = \mathbf{x}'\boldsymbol{\gamma} + \mathbf{x}'\boldsymbol{\eta} \cdot \varepsilon, \quad \varepsilon \perp \mathbf{x}.$

$$\implies q_{\tau}(y \mid \mathbf{x}) = \mathbf{x}'[\boldsymbol{\gamma} + \boldsymbol{\eta} \cdot q_{\tau}(\varepsilon)].$$

(Having  $\mathbf{x}$  in both mean and standard deviation is not a real restriction, i.e., set  $\mathbf{x} = (\mathbf{z}, \mathbf{w})$ ,

$$\boldsymbol{\gamma} = (\boldsymbol{\gamma}_z, \mathbf{0}), \boldsymbol{\eta} = (\mathbf{0}, \boldsymbol{\eta}_w).$$

# Quantile Regression

## Examples

3. **Fixed-Quantile Error:**  $y = \mathbf{x}'\beta + \varepsilon$ , where  $\varepsilon$  is not independent of  $\mathbf{x}$ , but

$$q_{\tau}(\varepsilon \mid \mathbf{x}) = \text{CONST.}$$

For example,  $\varepsilon \mid \mathbf{x} \sim \sigma_{\mathbf{x}} \cdot t_{(\nu_{\mathbf{x}})}$ , where  $\nu_{\mathbf{x}}$  is arbitrary and

$$\sigma_{\mathbf{x}} = \frac{\text{CONST}}{\text{qt}(\tau, \text{df} = \nu_{\mathbf{x}})}$$

# Quantile Regression

## Examples

4. **Fully specified QR model:**  $q_\tau(y | \mathbf{x}) = \mathbf{x}'\boldsymbol{\beta}_\tau$  for all  $0 < \tau < 1$ .

Actually quite restrictive since quantiles need to be ordered:

$$\tau_1 < \tau_2 \quad \implies \quad \mathbf{x}'\boldsymbol{\beta}_{\tau_1} < \mathbf{x}'\boldsymbol{\beta}_{\tau_2} \quad \forall \mathbf{x} \in \mathbb{R}^p.$$

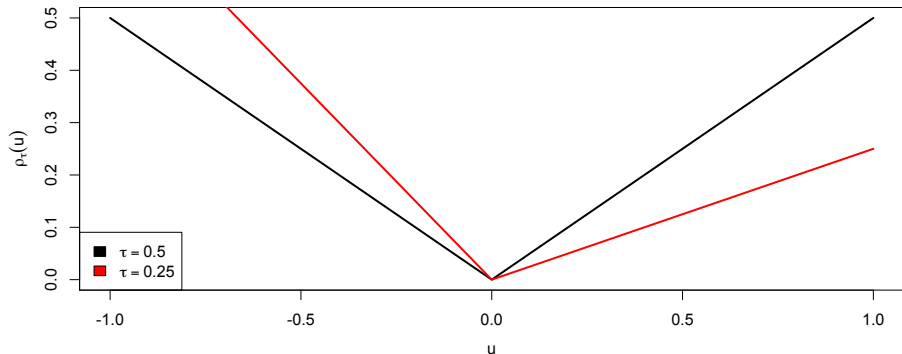


# Parameter Estimation

► **Quantile Regression Model:**  $q_\tau(y \mid \mathbf{x}) = \mathbf{x}'\boldsymbol{\beta}$  for given  $\tau \in (0, 1)$ .

► **Moment Condition:** If true parameter value if  $\boldsymbol{\beta} = \boldsymbol{\beta}_0$ , then

$$\boldsymbol{\beta}_0 = \arg \min_{\boldsymbol{\beta}} E[\rho_\tau(y - \mathbf{x}'\boldsymbol{\beta})], \quad \rho_\tau(u) = u \cdot (\tau - \mathbb{1}\{u < 0\}).$$



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► **Sample Analog:**

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \sum_{i=1}^n \rho_\tau(y_i - \mathbf{x}'_i\boldsymbol{\beta}).$$

# Parameter Estimation

► **Quantile Regression Model:**  $q_\tau(\alpha \mid \mathbf{x}) = \mathbf{x}'\boldsymbol{\beta}$  for given  $\tau \in (0, 1)$ .

► **Point Estimate:**

$$\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \sum_{i=1}^n \rho_\tau(y_i - \mathbf{x}'_i \boldsymbol{\beta}), \quad \rho_\tau(u) = u \cdot (\tau - \mathbb{1}\{u < 0\}).$$

**Equivalent Formulation:**

$$\min_{\boldsymbol{\beta}^+, \boldsymbol{\beta}^-, \mathbf{u}^+, \mathbf{u}^-} \sum_{i=1}^n \tau u_i^+ + (1-\tau) u_i^- \quad \text{subject to} \quad \mathbf{X}(\boldsymbol{\beta}^+ - \boldsymbol{\beta}^-) + \mathbf{u}^+ - \mathbf{u}^- = \mathbf{y},$$

where  $\beta_j^+ = \max(\beta_j, 0)$ ,  $\beta_j^- = -\min(\beta_j, 0)$  and similarly for  $u_i^+$  and  $u_i^-$ .

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where  $\beta_j^+ = \max(\beta_j, 0)$ ,  $\beta_j^- = -\min(\beta_j, 0)$  and similarly for  $u_i^+$  and  $u_i^-$ .

This is a **linear program** in  $\mathbf{w} = (\boldsymbol{\beta}^+, \boldsymbol{\beta}^-, \mathbf{u}^+, \mathbf{u}^-)$ ,

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w}} \mathbf{c}'\mathbf{w} \quad \text{subject to} \quad \mathbf{A}\mathbf{w} \leq \mathbf{b}, \mathbf{w} \geq \mathbf{0},$$

for which [efficient algorithms](#) are available.

# Quantile Regression

- ▶ **Model:**  $q_\tau(y | \mathbf{x}) = \mathbf{x}'\boldsymbol{\beta}$  for given  $\tau \in (0, 1)$ .
- ▶ **Point Estimate:**  $\hat{\boldsymbol{\beta}} = \arg \min_{\boldsymbol{\beta}} \sum_{i=1}^n \rho_\tau(y_i - \mathbf{x}'_i \boldsymbol{\beta})$  via linear programming.
- ▶ **Confidence Intervals:** ???, since we don't have a likelihood to calculate Observed Fisher Information!
  - ▶ Add modeling assumptions  $\implies \hat{\boldsymbol{\beta}} \rightarrow \mathcal{N}(\boldsymbol{\beta}_0, \boldsymbol{\Sigma})$ , but  $\boldsymbol{\Sigma}$  is difficult to estimate (nonparametric smoothing estimator with high variance).
  - ▶ Can do something much simpler... (but computationally more intensive)

# The Problem

- ▶ **Data and Model:**  $\mathbf{y} = (y_1, \dots, y_n) \sim F(\mathbf{y})$ .

I.e., completely general data-generating process (DGP) on the random vector  $\mathbf{y}$ . Could be a parametric model  $\mathbf{y} \sim f(\mathbf{y} | \boldsymbol{\theta})$ , a nonparametric model  $y_i \stackrel{\text{iid}}{\sim} F(y)$ , or a semi-parametric model like quantile regression...

- ▶ **Quantity of Interest:**  $\tau_0 = \mathcal{G}(F)$ .

I.e.,  $\tau_0$  must be some functional of the DGP. Could be  $\tau_0 = \tau(\boldsymbol{\theta}_0)$ , or the median of  $F$ ...

- ▶ **Estimator:**  $\hat{\tau} = g(\mathbf{y})$ .

- ▶ **Objective:** Calculate a confidence interval for  $\tau_0$ .

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- ▶ **Quantity of Interest:**  $\tau_0 = \mathcal{G}(F)$ .
- ▶ **Estimator:**  $\hat{\tau} = g(\mathbf{y})$ .
- ▶ **Objective:** Calculate a confidence interval for  $\tau_0$ .
- ▶ **Problem:** Can't use likelihood theory because:
  1. Don't have a parametric likelihood  $f(\mathbf{y} | \boldsymbol{\theta})$ .
  2. Have likelihood but estimator is not MLE (e.g., lasso for variable selection).
  3. Have likelihood + MLE, but suspect some degree of model misspecification.
  4. Have likelihood + MLE + correct model, but sample size  $n$  is too small for asymptotics to kick in.

# The Bootstrap Method

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 $\mathbf{y} = (y_1, \dots, y_n) \sim F(\mathbf{y})$ .
- ▶ **Quantity of Interest:**  $\tau_0 = \mathcal{G}(F)$ .
- ▶ **Estimator:**  $\hat{\tau} = g(\mathbf{y})$ .
- ▶ **Objective:** Calculate a confidence interval for  $\tau_0$ .
- ▶ **Idealized Scenario:** Suppose an **oracle** gives you the distribution of the **pivotal quantity**  $T = \tau_0 - \hat{\tau}$ . Then

$$\Pr(L < T < U) = \Pr(L < \tau_0 - \hat{\tau} < U) = \Pr(\hat{\tau} + L < \tau_0 < \hat{\tau} + U).$$

$\implies$  If  $L/U$  are the 2.5/97.5% quantiles of  $T$ , then a 95% CI for  $\tau_0$  is

$$\tau_0 \in (\hat{\tau} + L, \hat{\tau} + U).$$



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- ▶ **Estimator:**  $\hat{\tau} = g(\mathbf{y})$ .
- ▶ **Oracle:** Suppose distribution of  $T = \tau_0 - \hat{\tau}$  is given.  
If  $L/U$  are the 2.5/97.5% quantiles of  $T$ , then CI for  $\tau_0$  is  $(\hat{\tau} + L, \hat{\tau} + U)$ .
- ▶ **Bootstrap:** Estimate  $L$  and  $U$  as follows:
  1. **Simulate**  $M$  datasets  $\tilde{\mathbf{y}}^{(m)} \stackrel{\text{iid}}{\sim} \hat{F}(\mathbf{y})$ , each of size  $n$ , where  $\hat{F}(\mathbf{y})$  is an estimate of  $F(\mathbf{y})$ . The two most common ways to do this are:
    - i. **Parametric Bootstrap:** If  $\mathbf{y} \sim f(\mathbf{y} \mid \boldsymbol{\theta})$ , then  $\tilde{\mathbf{y}}^{(m)} \stackrel{\text{iid}}{\sim} f(\mathbf{y} \mid \hat{\boldsymbol{\theta}})$ .
    - ii. **Nonparametric Bootstrap:** If  $y_i \stackrel{\text{iid}}{\sim} F(y)$ , then  $y_i^{(m)} \stackrel{\text{iid}}{\sim} \hat{F}(y)$ , where  $\hat{F}(y)$  is the empirical CDF of  $\mathbf{y}$ . In other words,  $\tilde{\mathbf{y}}^{(m)}$  is sampled  $n$  times with replacement from  $\mathbf{y}$ .

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  2. For each dataset, calculate  $\tilde{\tau}^{(m)} = g(\tilde{\mathbf{y}}^{(m)})$  and  $\tilde{T}^{(m)} = \hat{\tau} - \tilde{\tau}^{(m)}$ .

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  3. Let  $\tilde{L}/\tilde{U}$  be the 2.5/97% *sample* quantiles of  $\tilde{T}^{(1)}, \dots, \tilde{T}^{(M)}$ .

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  2. For each dataset, calculate  $\tilde{\tau}^{(m)} = g(\tilde{\mathbf{y}}^{(m)})$  and  $\tilde{T}^{(m)} = \hat{\tau} - \tilde{\tau}^{(m)}$ .
  3. Let  $\tilde{L}/\tilde{U}$  be the 2.5/97% *sample* quantiles of  $\tilde{T}^{(1)}, \dots, \tilde{T}^{(M)}$ .  
 $\implies$  The Bootstrap CI for  $\tau_0$  is given by  $(\hat{\tau} + \tilde{L}, \hat{\tau} + \tilde{U})$ .

# The Bootstrap Method

	Real World	Bootstrap World
Sampling Distribution	$\mathbf{y} \sim F(\mathbf{y})$	$\tilde{\mathbf{y}} \sim \hat{F}(\mathbf{y})$
Quantity of Interest	$\tau_0 = \mathcal{G}(F)$	$\hat{\tau} = g(\mathbf{y})$
Estimator	$\hat{\tau} = g(\mathbf{y})$	$\tilde{\tau} = g(\tilde{\mathbf{y}})$
Pivotal Quantity	$T = \tau_0 - \hat{\tau}$	$\tilde{T} = \hat{\tau} - \tilde{\tau}$
Quantiles:	$P(L < T < U) = 95\%$	$P(\tilde{L} < \tilde{T} < \tilde{U}) = 95\%$
95% Confidence Interval	Oracle: $(\hat{\tau} + L, \hat{\tau} + U)$ Bootstrap: $(\hat{\tau} + \tilde{L}, \hat{\tau} + \tilde{U})$	

Parallel between the **Real** world and the **Bootstrap** world.

## Example: Range of Uniform

- ▶ **Objective:** Given  $\mathbf{U} = (U_1, \dots, U_n)$ ,  $U_i \stackrel{\text{iid}}{\sim} \text{Unif}(0, \theta)$ , we wish to estimate  $\theta$ .
- ▶ **Simulation Study:** Generate  $N = 1000$  datasets with  $\theta_0 = 1$  and perform calculations for each of the following settings:

2. *Estimators:* (i) MLE  $\hat{\theta}_1 = \max(\mathbf{U})$  and (ii) Unbiased  $\hat{\theta}_2 = 2\bar{\mathbf{U}}$  (since  $E[\bar{\mathbf{U}}] = \theta/2$ ).

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  3. *Bootstrap Sampling:* (i) Nonparametric ( $\tilde{\mathbf{U}}$  sampled with replacement) and (ii) Parametric ( $\tilde{U}_i^{(m)} \stackrel{\text{iid}}{\sim} \text{Unif}(0, \hat{\theta})$ ). Always use  $M = 1000$  bootstrap samples.



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  4. *Confidence Intervals:* (i) Basic Bootstrap:  $(\hat{\theta} + \tilde{L}, \hat{\theta} + \tilde{U})$   
(ii) Percentile Bootstrap 2.5/97.5% quantiles of  $\tilde{\theta}^{(1)}, \dots, \tilde{\theta}^{(M)}$ . (seems simpler but...)

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  5. *Model Misspecification:* True sampling distribution is  $U_i \stackrel{\text{iid}}{\sim} \theta \times \text{Beta}(\alpha, \alpha)$ , where (i)  $\alpha = 1$  ( $\text{Beta}(1, 1) = \text{Unif}(0, 1)$ ) and (ii)  $\alpha = 2$ .  
( $\theta$  is range of distribution, so still meaningful quantity to estimate. For  $\alpha \neq 1$ ,  $\hat{\theta}_1$  no longer MLE, but  $\hat{\theta}_2$  still unbiased.)

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- ▶ **Simulation Study:** For  $N = 1000$  datasets with  $\theta_0 = 1$ :
  1. *Sample Size:* (i)  $n = 100$  and (ii)  $n = 10000$
  2. *Estimators:* (i)  $\hat{\theta}_1 = \max(\mathbf{U})$  and (ii)  $\hat{\theta}_2 = 2\bar{\mathbf{U}}$ .
  3. *Bootstrap Sampling:* For  $M = 1000$  bootstrap samples, sampling is
    - i. Nonparametric:  $\tilde{\mathbf{U}}$  sampled with replacement.

Variance Reduction Use same  $\tilde{\mathbf{U}}^{(m)}$  to calculate both  $\hat{\theta}_1^{(m)}$  and  $\hat{\theta}_2^{(m)}$ .  
 $\implies$  Monte Carlo *difference* between comparison metrics has same expectation, but lower variance
    - ii. Parametric:  $\tilde{U}_i^{(m)} \stackrel{\text{iid}}{\sim} \text{Unif}(0, \hat{\theta})$ .
  4. *Confidence Intervals:* (i) Basic Bootstrap and (ii) Percentile Bootstrap.
  5. *Model Misspecification:*  $U_i \stackrel{\text{iid}}{\sim} \theta \times \text{Beta}(\alpha, \alpha)$ , where (i)  $\alpha = 1$  and (ii)  $\alpha = 2$ .
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- ▶ **Simulation Study:** For  $N = 1000$  datasets with  $\theta_0 = 1$ :
  1. *Sample Size:* (i)  $n = 100$  and (ii)  $n = 10000$
  2. *Estimators:* (i)  $\hat{\theta}_1 = \max(\mathbf{U})$  and (ii)  $\hat{\theta}_2 = 2\bar{\mathbf{U}}$ .
  3. *Bootstrap Sampling:* For  $M = 1000$  bootstrap samples, sampling is
    - i. Nonparametric:  $\tilde{\mathbf{U}}$  sampled with replacement.

**Variance Reduction** Use same  $\tilde{\mathbf{U}}^{(m)}$  to calculate both  $\hat{\theta}_1^{(m)}$  and  $\hat{\theta}_2^{(m)}$ .
    - ii. Parametric:  $\tilde{U}_i^{(m)} \stackrel{\text{iid}}{\sim} \text{Unif}(0, \hat{\theta})$ .

**Variance Reduction** Use same  $\tilde{R}_i^{(m)} \stackrel{\text{iid}}{\sim} \text{Unif}(0, 1)$ , and let  $\tilde{U}_i^{(m)} = \hat{\theta}_k \tilde{R}_i^{(m)}$ ,  $k = 1, 2$ .
  4. *Confidence Intervals:* (i) Basic Bootstrap and (ii) Percentile Bootstrap.
  5. *Model Misspecification:*  $U_i \stackrel{\text{iid}}{\sim} \theta \times \text{Beta}(\alpha, \alpha)$ , where (i)  $\alpha = 1$  and (ii)  $\alpha = 2$ .
- ▶ **Comparison Metrics:** (i) True coverage of CI and (ii) Average width of CI.

# Example: Range of Uniform

## Actual Coverage

alpha = 1

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.86	0.94	0.94	0.95
basic_n=10K	0.89	0.95	0.95	0.94
pct_n=100	0.00	0.95	0.00	0.95
pct_n=10K	0.00	0.95	0.00	0.95

alpha = 2

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.60	0.93	0.29	0.98
basic_n=10K	0.57	0.95	0.00	0.98
pct_n=100	0.00	0.94	0.00	0.98
pct_n=10K	0.00	0.95	0.00	0.99

## Interval Width

alpha = 1

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.03	0.22	0.04	0.22
basic_n=10K	0.00	0.02	0.00	0.02
pct_n=100	0.03	0.22	0.04	0.22
pct_n=10K	0.00	0.02	0.00	0.02

alpha = 2

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.07	0.17	0.03	0.22
basic_n=10K	0.01	0.02	0.00	0.02
pct_n=100	0.07	0.17	0.03	0.22
pct_n=10K	0.01	0.02	0.00	0.02

## Remarks:

1. Percentile CI based on  $\hat{\theta}_1 = \max(\mathbf{U})$  has 0% coverage! This is because  $\theta_0 > \hat{\theta}_1 > \tilde{\theta}_1^{(m)}$ , so quantiles of  $\tilde{\theta}_1^{(m)}$  can never cover  $\theta_0$ .

# Example: Range of Uniform

## Actual Coverage

alpha = 1

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.86	0.94	0.94	0.95
basic_n=10K	0.89	0.95	0.95	0.94
pct_n=100	0.00	0.95	0.00	0.95
pct_n=10K	0.00	0.95	0.00	0.95

alpha = 2

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.60	0.93	0.29	0.98
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pct_n=10K	0.00	0.95	0.00	0.99

## Interval Width

alpha = 1

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.03	0.22	0.04	0.22
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basic_n=100	0.07	0.17	0.03	0.22
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pct_n=100	0.07	0.17	0.03	0.22
pct_n=10K	0.01	0.02	0.00	0.02

## Remarks:

2. NP bootstrap with Basic CI does not approach 95% coverage as sample size  $n \rightarrow \infty$ ! This is because bootstrap only works if  $\tilde{\theta}$  and  $\hat{\theta}$  have the same distribution as  $n \rightarrow \infty$ . However,  $\hat{\theta}_1 \sim \theta_0 \times \text{Beta}(1, n)$  is a continuous distribution, but

$$\Pr(\tilde{\theta}_1 = \hat{\theta}_1) = 1 - \Pr(\tilde{\theta}_1 \neq \hat{\theta}_1) = 1 - (1 - \frac{1}{n})^n \rightarrow 1 - e^{-1} \approx 0.63.$$

Therefore,  $\tilde{\theta}_1$  has a non-vanishing point mass at  $\hat{\theta}_1$ , so doesn't get close to continuous distribution of  $\hat{\theta}_1$ .

# Example: Range of Uniform

## Actual Coverage

alpha = 1

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.86	0.94	0.94	0.95
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alpha = 2

	NP_max	NP_mean2	P_max	P_mean2
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pct_n=100	0.00	0.94	0.00	0.98
pct_n=10K	0.00	0.95	0.00	0.99

## Interval Width

alpha = 1

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.03	0.22	0.04	0.22
basic_n=10K	0.00	0.02	0.00	0.02
pct_n=100	0.03	0.22	0.04	0.22
pct_n=10K	0.00	0.02	0.00	0.02

alpha = 2

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.07	0.17	0.03	0.22
basic_n=10K	0.01	0.02	0.00	0.02
pct_n=100	0.07	0.17	0.03	0.22
pct_n=10K	0.01	0.02	0.00	0.02

## Remarks:

- NP-CI for  $\hat{\theta}_2$  have the right coverage, even under wrong model  $\alpha = 2$ . On the other hand P-CI with  $\hat{\theta}_2$  overcover under wrong model (98% instead of 95%).



# Example: Range of Uniform

## Actual Coverage

alpha = 1

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.86	0.94	0.94	0.95
basic_n=10K	0.89	0.95	0.95	0.94
pct_n=100	0.00	0.95	0.00	0.95
pct_n=10K	0.00	0.95	0.00	0.95

alpha = 2

	NP_max	NP_mean2	P_max	P_mean2
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## Interval Width

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	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.03	0.22	0.04	0.22
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pct_n=100	0.03	0.22	0.04	0.22
pct_n=10K	0.00	0.02	0.00	0.02

alpha = 2

	NP_max	NP_mean2	P_max	P_mean2
basic_n=100	0.07	0.17	0.03	0.22
basic_n=10K	0.01	0.02	0.00	0.02
pct_n=100	0.07	0.17	0.03	0.22
pct_n=10K	0.01	0.02	0.00	0.02

## Remarks:

- $\hat{\theta}_1$  does not converge to  $\theta_0$  under the wrong model  $\alpha = 2$ , so CI has poor coverage. On the other hand, interval width is narrower than with  $\hat{\theta}_2$ , because max has less variance than mean.

# Example: GARCH Stochastic Volatility Model

- ▶ **SDE SV Model:** Let  $(\Delta X_t, \Delta V_t)$  be the asset/volatility log-return/return on day  $t$ . The basic SDE-SV model is

$$\Delta X_t = \left(\alpha - \frac{1}{2} V_t\right) \Delta t + V_t^{1/2} \Delta B_{1t}$$

$$\Delta V_t = -\gamma(V_t - \mu) \Delta t + \sigma V_t^{1/2} \Delta B_{2t}$$

- ▶ **Pros:** Excellent performance; easy to calibrate when  $V_t$  is observed (e.g., VIX for GSPC).
- ▶ **Cons:** Extremely difficult to calibrate when  $V_t$  is **latent**, since  $\ell(\boldsymbol{\theta} | \mathbf{X})$  is not available in closed-form, i.e.,

$$\mathcal{L}(\boldsymbol{\theta} | \mathbf{X}) \propto p(\mathbf{X} | \boldsymbol{\theta}) = \int p(\mathbf{X}, \mathbf{V} | \boldsymbol{\theta}) d\mathbf{V}$$

# GARCH Stochastic Volatility Model

► SDE SV Model:

$$\Delta X_t = (\alpha - \frac{1}{2} V_t) \Delta t + V_t^{1/2} \Delta B_{1t}$$

$$\Delta V_t = -\gamma(V_t - \mu) \Delta t + \sigma V_t^{1/2} \Delta B_{2t}$$

► GARCH SV Model: Let  $\varepsilon_t = \Delta X_t$ . The GARCH(1,1) model is

$$\varepsilon_t = \sigma_t z_t, \quad z_t \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$$

$$\sigma_t^2 = \omega + \alpha \varepsilon_{t-1}^2 + \beta \sigma_{t-1}^2$$

- Like SDEs, volatility  $\sigma_t$  is stochastic.
- **Pros:** Inference with GARCH is far simpler than with SDE (closed-form likelihood).
- **Cons:** Unlike SDEs, GARCH is a discrete-time model (difficult for option pricing and consistency across timescales)

# GARCH Stochastic Volatility Model

- ▶ **Data:** Asset values  $\mathbf{S} = (S_0, \dots, S_N) \implies$  log-returns  $\boldsymbol{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_N)$ , with  $\varepsilon_t = \log(S_t/S_{t-1})$ .
- ▶ **GARCH(1,1) Model:** 
$$\varepsilon_t = \sigma_t z_t, \quad z_t \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$$
$$\sigma_t^2 = \omega + \alpha \varepsilon_{t-1}^2 + \beta \sigma_{t-1}^2$$
- ▶ **Objective:** On given day  $N$ , estimate the  $p$ -day forward  $\tau$ -level **Value-At-Risk**, i.e., the conditional quantile

$$\text{VaR}_\tau = q_\tau \left( \frac{S_{N+p} - S_N}{S_N} \mid \mathbf{S}, \boldsymbol{\theta} \right) \iff \Pr \left( \frac{S_{N+p} - S_N}{S_N} < \text{VaR}_\tau \mid \mathbf{S}, \boldsymbol{\theta} \right) = \tau.$$

For example, we would say that the 10-day 5%-level VaR of AAPL is a 1.3% drop in value.

# GARCH Model

► **Model:**  $\varepsilon_t = \sigma_t z_t, \quad z_t \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$   
 $\sigma_t^2 = \omega + \alpha \varepsilon_{t-1}^2 + \beta \sigma_{t-1}^2$

► **Parameter Estimation:**

► *R Packages* **rugarch**, **fGarch**. The former is more stable, the latter is faster. Both can fit numerous extensions to the basic GARCH(1,1) model above.

► *Profile Likelihood* For  $\theta = (\omega, \alpha, \beta)$

$$\begin{aligned} \ell(\theta \mid \varepsilon) &= -\frac{1}{2} \sum_{t=1}^N \frac{\varepsilon_t^2}{\sigma_t^2} + \log(\sigma_t^2), & \sigma_t^2 &= \omega + \alpha \varepsilon_{t-1}^2 + \beta \sigma_{t-1}^2 \\ &= -\frac{1}{2} \sum_{t=1}^N \frac{\varepsilon_t^2}{\omega \cdot \tilde{\sigma}_t^2} + \log(\omega \cdot \tilde{\sigma}_t^2), & \tilde{\sigma}_t^2 &= 1 + \eta \varepsilon_{t-1}^2 + \beta \tilde{\sigma}_{t-1}^2, \end{aligned}$$

where  $\eta = \alpha/\omega \implies \hat{\omega}(\eta, \beta) = \sum_{t=1}^N (\varepsilon_t / \tilde{\sigma}_t)^2$ .

(Note the technical issue of initializing  $\tilde{\sigma}_1$  which we won't discuss here.)

# Value-at-Risk

► **GARCH(1,1) Model:**  $\varepsilon_t = \sigma_t z_t, \quad z_t \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$   
 $\sigma_t^2 = \omega + \alpha \varepsilon_{t-1}^2 + \beta \sigma_{t-1}^2$

► **Value-at-Risk:**

$$\text{VaR}_\tau = q_\tau \left( \frac{S_{N+p} - S_N}{S_N} \mid \mathbf{S}, \boldsymbol{\theta} \right) \iff \Pr \left( \frac{S_{N+p} - S_N}{S_N} < \text{VaR}_\tau \mid \mathbf{S}, \boldsymbol{\theta} \right) = \tau.$$

► **1-Day VaR:** For given  $\boldsymbol{\theta}$  and data  $\boldsymbol{\varepsilon} = (\varepsilon_1, \dots, \varepsilon_N)$

1. Let  $\sigma_1^2 = E[\sigma_1^2 \mid \boldsymbol{\theta}] = \omega / (1 - \alpha - \beta)$
2. Use GARCH equation to obtain  $\sigma_{N+1}^2 = \omega + \alpha \varepsilon_N^2 + \beta \sigma_N^2$
3.  $(S_{N+1} - S_N) / S_N = \exp(\varepsilon_{N+1}) - 1 \implies \text{VaR}_\tau = \exp\{\text{qnorm}(\tau \mid 0, \sigma_{N+1})\} - 1$

In other words,  $\text{VaR}_\tau = \text{VaR}_\tau(\boldsymbol{\theta} \mid \boldsymbol{\varepsilon})$  is a function of  $\boldsymbol{\theta}$  (and observed data  $\boldsymbol{\varepsilon}$ ).

# Value-at-Risk

► **GARCH(1,1) Model:**  $\varepsilon_t = \sigma_t z_t, \quad z_t \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$   
 $\sigma_t^2 = \omega + \alpha \varepsilon_{t-1}^2 + \beta \sigma_{t-1}^2$

► **1-Day VaR:** For given  $\theta$  and data  $\varepsilon = (\varepsilon_1, \dots, \varepsilon_N)$

1. Let  $\sigma_1^2 = E[\sigma_1^2 | \theta] = \omega / (1 - \alpha - \beta)$

2. Use GARCH equation to obtain  $\sigma_{N+1}^2 = \omega + \alpha \varepsilon_N^2 + \beta \sigma_N^2$

3.  $(S_{N+1} - S_N) / S_N = \exp(\varepsilon_{N+1}) - 1 \implies \text{VaR}_\tau = \exp\{\text{qnorm}(\tau | 0, \sigma_{N+1})\} - 1$

In other words,  $\text{VaR}_\tau = \text{VaR}_\tau(\theta | \varepsilon)$ .

► **Inference:** If  $\hat{\theta}$  is the MLE of GARCH model, then

► *MLE:* Use **plug-in** principle:  $\hat{\text{VaR}}_\tau = \text{VaR}_\tau(\hat{\theta} | \varepsilon)$ .

► *Confidence Intervals?*

# Delta-Method

- ▶ **Data-Generating Process:** Let  $Y_1, Y_2, \dots$  be some stochastic process determined by a parameter  $\theta \in \mathbb{R}^p$

(In the simplest case, we have  $Y_n \stackrel{\text{iid}}{\sim} f(y | \theta)$ , but the theory works for stationary processes such as GARCH(1,1) as well).

- ▶ **Asymptotic Normality:** For  $\mathbf{Y}_{1:n} = (Y_1, \dots, Y_n)$ , suppose the MLE and the inverse Fisher Information

$$\hat{\theta}_n = \arg \max_{\theta} \ell(\theta | \mathbf{Y}_{1:n}), \quad \hat{\mathbf{V}}_n = \left[ -\frac{\partial^2}{\partial \theta^2} \ell(\theta | \mathbf{Y}_{1:n}) \right]^{-1}$$

satisfy the usual asymptotic theory, i.e.,  $\hat{\mathbf{V}}_n^{1/2}(\hat{\theta}_n - \theta_0) \rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I}_p)$  as  $n \rightarrow \infty$ , where  $\theta_0$  is the true parameter value.



# Delta-Method

**Theorem:** Let  $\hat{\theta}_n$  be a sequence of estimators such that as  $n \rightarrow \infty$  we have

$$\hat{\mathbf{V}}_n^{1/2}(\hat{\theta}_n - \theta_0) \rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I}).$$

Suppose that  $\tau : \mathbb{R}^p \rightarrow \mathbb{R}^q$  is a continuously differentiable function with  $q \leq p$ , and we wish to estimate  $\tau_0 = \tau(\theta_0)$ . Then as  $n \rightarrow \infty$  we have

$$\begin{aligned} \hat{\Sigma}_n^{1/2}(\hat{\tau}_n - \tau_0) &\rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I}), & \hat{\tau}_n &= \tau(\hat{\theta}_n) \\ \hat{\Sigma}_n &= [\nabla \tau(\hat{\theta}_n)]' \hat{\mathbf{V}}_n [\nabla \tau(\hat{\theta}_n)]. \end{aligned}$$

# Delta-Method

**Theorem:** Let  $\hat{\theta}_n$  be a sequence of estimators such that as  $n \rightarrow \infty$  we have

$$\hat{\mathbf{V}}_n^{1/2}(\hat{\theta}_n - \theta_0) \rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I}).$$

Suppose that  $\tau : \mathbb{R}^p \rightarrow \mathbb{R}^q$  is a continuously differentiable function with  $q \leq p$ , and we wish to estimate  $\tau_0 = \tau(\theta_0)$ . Then as  $n \rightarrow \infty$  we have

$$\hat{\Sigma}_n^{1/2}(\hat{\tau}_n - \tau_0) \rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \hat{\tau}_n = \tau(\hat{\theta}_n)$$
$$\hat{\Sigma}_n = [\nabla \tau(\hat{\theta}_n)]' \hat{\mathbf{V}}_n [\nabla \tau(\hat{\theta}_n)].$$

*Proof:* The 1st order Taylor expansion of  $\tau(\hat{\theta}_n)$  about  $\theta = \theta_0$  gives

$$\tau(\hat{\theta}_n) - \tau(\theta_0) \approx [\nabla \tau(\theta_0)]'(\hat{\theta}_n - \theta_0).$$

Since  $\hat{\theta}_n - \theta_0 \approx \mathcal{N}(\mathbf{0}, \hat{\mathbf{V}}_n)$ , by linearity of MVN we have

$$\hat{\tau}_n - \tau_0 \approx \mathcal{N}(\mathbf{0}, [\nabla \tau(\theta_0)]' \hat{\mathbf{V}}_n [\nabla \tau(\theta_0)]).$$

# Delta-Method

- **Theorem:** If  $\hat{\mathbf{V}}_n^{1/2}(\hat{\boldsymbol{\theta}}_n - \boldsymbol{\theta}_0) \rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I})$  and  $\tau : \mathbb{R}^p \rightarrow \mathbb{R}^q$  is a continuously differentiable function with  $q \leq p$ , then

$$\hat{\boldsymbol{\Sigma}}_n^{1/2}(\hat{\boldsymbol{\tau}}_n - \boldsymbol{\tau}_0) \rightarrow \mathcal{N}(\mathbf{0}, \mathbf{I}), \quad \hat{\boldsymbol{\tau}}_n = \tau(\hat{\boldsymbol{\theta}}_n)$$
$$\hat{\boldsymbol{\Sigma}}_n = [\nabla \tau(\hat{\boldsymbol{\theta}}_n)]' \hat{\mathbf{V}}_n [\nabla \tau(\hat{\boldsymbol{\theta}}_n)].$$

- **Upshot:** If  $(\hat{\boldsymbol{\theta}}, \hat{\mathbf{V}})$  are the MLE and its variance estimator, a confidence interval for a 1D quantity of interest  $\tau_0 = \tau(\boldsymbol{\theta}_0)$  can be constructed via

$$\hat{\tau} \pm 1.96 \cdot s_{\hat{\tau}}, \quad \hat{\tau} = \tau(\hat{\boldsymbol{\theta}})$$
$$s_{\hat{\tau}} = \sqrt{[\nabla \tau(\hat{\boldsymbol{\theta}})]' \hat{\mathbf{V}} [\nabla \tau(\hat{\boldsymbol{\theta}})]}.$$

Can use this to calculate CI for 1-day  $\text{VaR}_{\tau} = \tau(\boldsymbol{\theta}_0) = \text{VaR}_{\tau}(\boldsymbol{\theta}_0 \mid \varepsilon)$ .

# Value-at-Risk

► **GARCH(1,1) Model:**  $\varepsilon_t = \sigma_t z_t, \quad z_t \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$   
 $\sigma_t^2 = \omega + \alpha \varepsilon_{t-1}^2 + \beta \sigma_{t-1}^2$

► **Value-at-Risk:**

$$\text{VaR}_\tau = q_\tau \left( \frac{S_{N+p} - S_N}{S_N} \mid \mathbf{s}, \boldsymbol{\theta} \right) \iff \Pr \left( \frac{S_{N+p} - S_N}{S_N} < \text{VaR}_\tau \mid \mathbf{s}, \boldsymbol{\theta} \right) = \tau.$$

No analytic solution for  $p > 1$ .

► **Point Estimate:** Use Monte Carlo:

1. For given  $\boldsymbol{\theta}$ , analytically obtain  $\sigma_1^2, \dots, \sigma_N^2$ .
2. Generate  $M$  iid realizations of  $R = \log(S_{N+p}/S_N)$  from  $p(R \mid \varepsilon_N, \sigma_N)$  using GARCH. (Note that  $R = \sum_{i=1}^p \varepsilon_{N+i}$ )
3. The Monte Carlo approximation is  $\text{VaR}_\tau = \exp\{\hat{q}_\tau(R \mid \varepsilon_N, \boldsymbol{\theta})\} - 1$ , where  $\hat{q}_\tau(R \mid \varepsilon_N, \boldsymbol{\theta})$  is the  $\tau$ -level sample quantile of the iid realizations  $R^{(1)}, \dots, R^{(M)}$ .

► **Interval Estimate:** Use Delta-Method, with  $\hat{\text{VaR}}_\tau = \exp\{\hat{q}_\tau(R \mid \varepsilon_N, \hat{\boldsymbol{\theta}})\} - 1$ , but with **variance reduction**, i.e., same  $z_{N+1}^{(m)}, \dots, z_{N+p}^{(m)}$  for every value of  $\boldsymbol{\theta}$ .

# Value-at-Risk

- ▶ **GARCH(1,1) Model:**  $\varepsilon_t = \sigma_t z_t, \quad z_t \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$   
 $\sigma_t^2 = \omega + \alpha \varepsilon_{t-1}^2 + \beta \sigma_{t-1}^2$

- ▶ **Value-at-Risk:**

$$\text{VaR}_\tau = q_\tau \left( \frac{S_{N+p} - S_N}{S_N} \mid \mathbf{S}, \boldsymbol{\theta} \right) \iff \Pr \left( \frac{S_{N+p} - S_N}{S_N} < \text{VaR}_\tau \mid \mathbf{S}, \boldsymbol{\theta} \right) = \tau.$$

- ▶ **Point/Interval Estimate:** Monte Carlo + Delta Method
- ▶ **Model Misspecification:** Suppose we have GARCH(1,1), but with  $z_t \stackrel{\text{iid}}{\sim} F(z)$  with  $F \neq \mathcal{N}(0, 1)$ ?
- ▶ **Residual Bootstrap:**

- ▶ GARCH model:  $\varepsilon_t = \sigma_t z_t, \quad \sigma_t^2 = \omega + \alpha \varepsilon_{t-1}^2 + \beta \sigma_{t-1}^2$
- ▶ Use  $\hat{\boldsymbol{\theta}}$  to calculate  $\hat{\boldsymbol{\sigma}} = (\hat{\sigma}_1, \dots, \hat{\sigma}_N)$  and *residuals*  $\hat{\mathbf{z}} = (\hat{z}_1, \dots, \hat{z}_N) = \boldsymbol{\varepsilon} / \hat{\boldsymbol{\sigma}}$ .
- ▶ Obtain Bootstrap residuals  $\tilde{\mathbf{z}}$  by sampling with replacement from  $\hat{\mathbf{z}}$
- ▶ Bootstrap log-returns:  $\tilde{\varepsilon}_t = \tilde{\sigma}_t \tilde{z}_t, \quad \sigma_t^2 = \hat{\omega} + \hat{\alpha} + \tilde{\varepsilon}_{t-1}^2 + \hat{\beta} \tilde{\sigma}_{t-1}^2$