Parametric and Nonparametric Bootstrap Methods for General MANOVA

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Overview

- Multivariate data
  - Models
  - Limitations
- General MANOVA
  - Asymptotic tests
  - Resampling versions
- Summary
- References

Multivariate Data

- Occur frequently in practice
- More than one variable is observed per patient / subject
- Usual assumptions
  - Multivariate normality
  - Equal covariance matrices across the groups
  - Multivariate normality is quasi impossible to justify
- Multivariate data occur in factorial models
  - One-way layouts ($a = 4$ treatment groups, $p = 3$ endpoints)
  - Two-way factorial models (one-way layout with gender stratification)
  - ...
- Basically the same as ANOVA, but always one dimension more...

Data Layout

- Crossed designs
  - Example: Factor A with $a = 2$ levels, factor B with $b = 3$
  - Each vector $\mathbf{X}$ has p components (endpoints)

Factor B ($j = 1, 2, 3$)

Factor A ($i = 1, 2$)		$j = 1$	$j = 2$	$j = 3$
	$i = 1$	$\mathbf{X}_{111}$ ⋮ $\mathbf{X}_{11n_{11}}$	$\mathbf{X}_{121}$ ⋮ $\mathbf{X}_{12n_{12}}$	$\mathbf{X}_{131}$ ⋮ $\mathbf{X}_{13n_{13}}$
	$i = 2$	$\mathbf{X}_{211}$ ⋮ $\mathbf{X}_{21n_{21}}$	$\mathbf{X}_{221}$ ⋮ $\mathbf{X}_{22n_{22}}$	$\mathbf{X}_{231}$ ⋮ $\mathbf{X}_{23n_{23}}$

Factorial Designs

- $\mathbf{X}_{ijk} = \boldsymbol{\mu} + \boldsymbol{\alpha}_i + \boldsymbol{\beta}_j + \boldsymbol{\gamma}_{ij} + \boldsymbol{\epsilon}_{ijk}$
  - $i = 1, \ldots, a;\ j = 1, \ldots, b;\ k = 1, \ldots, n_{ij}$
  - $E(\boldsymbol{\epsilon}_{ijk}) = \mathbf{0},\ Var(\epsilon_{ijk}) = \boldsymbol{\Sigma}_{ij}$
  - Example: $i =$m,f; $j = 0, 1, 2, 3, 4$
- Hypotheses
  - No main effect A: $\boldsymbol{\alpha}_i = \mathbf{0}$
  - No main effect B: $\boldsymbol{\beta}_j = \mathbf{0}$
  - No interaction AB: $\boldsymbol{\gamma}_{ij} = \mathbf{0}$
- Simplification
  - $\boldsymbol{\mu} = (\mu_{11}, \ldots, \mu_{ab})'$
  - $H_0(A) : \mathbf{C}_A\boldsymbol{\mu} = \mathbf{0};\ H_0(B) : \mathbf{C}_B\boldsymbol{\mu} = \mathbf{0};\ H_0(AB) : \mathbf{C}_{AB}\boldsymbol{\mu} = \mathbf{0}$
  - Adequate matrices

Statistical Model

- Random vectors

$$\mathbf{X}_{ik} = \boldsymbol{\mu}_i + \boldsymbol{\epsilon}_{ik}, i = 1. \dots, a, ; k = 1, \dots, n_i.$$

- Error terms

$$\begin{aligned} E(\boldsymbol{\epsilon}_{ik}) &= 0, i = 1, \dots, a,\ k = 1, \dots, n_i, \\ Cov(\boldsymbol{\epsilon}_{ik}) &= \boldsymbol{\Sigma}_i > 0,\ i = 1, \dots, a,\ k = 1, \dots, n_i, \\ E(\|\boldsymbol{\epsilon}_{ik}\|^4) &< \infty,\ i = 1, \dots, a,\ k = 1, \dots, n_i. \end{aligned}$$

- Asymptotics: $N \to \infty :\ N/n_i \to \kappa_i < \infty$

Statistical Model - General MANOVA

- Re-arrangements

$$\begin{aligned} \mathbf{X} &= (\mathbf{X}'_{11}, \ldots, \mathbf{X}'_{an_a})' \\ \boldsymbol{\mu} &= (\boldsymbol{\mu}'_1, \ldots, \boldsymbol{\mu}'_d)' \\ \boldsymbol{\mu}_i &= (\mu_i^{(1)}, \ldots, \mu_i^{(p)})', \; i = 1, \ldots, a, \\ \boldsymbol{\epsilon} &= (\boldsymbol{\epsilon}'_{11}, \ldots, \boldsymbol{\epsilon}'_{an_a})'. \end{aligned}$$

General MANOVA: Hypotheses

- $H_0 : \mathbf{H}\boldsymbol{\mu} = \mathbf{0}$
  - Generalized Multivariate Behrens-Fisher problem: $H_0 : \mathbf{T}\boldsymbol{\mu} = \mathbf{0}$, $\mathbf{T} = \mathbf{P}_2 \otimes \mathbf{I}_p$
  - Multivariate one-way layout: $H_0 : \mathbf{T}\boldsymbol{\mu} = \mathbf{0}$, $\mathbf{T} = \mathbf{P}_a \otimes \mathbf{I}_p$
  - Crossed multivariate two-way layout with interactions: $H_0 : \mathbf{T}\boldsymbol{\mu} = \mathbf{0}$, $\mathbf{T} = \mathbf{P}_a \otimes \frac{1}{b}\mathbf{J}_b \otimes \mathbf{I}_p$
  - Hierarchically nested two-way design: $H_0 : \mathbf{T}\boldsymbol{\mu} = \mathbf{0}$, $\mathbf{T}$ appropriate

Estimators

- Point Estimates
  - Sample means: $\overline{\mathbf{X}}_{i\cdot} = \frac{1}{n_i}\sum_{k=1}^{n_i} \mathbf{X}_{ik}$
  - Mean vector: $\overline{\mathbf{X}}_{\cdot} = (\overline{\mathbf{X}}_{1\cdot}', \ldots, \overline{\mathbf{X}}_{d\cdot}')'$
  - Asymptotic distribution

$$\mathbf{V}_N = Cov(\sqrt{N}\ \overline{\mathbf{X}}_{\cdot}) \quad = \quad \operatorname{diag}\left(\frac{N}{n_i}\mathbf{\Sigma}_i : 1 \leq i \leq a\right).$$

  - Multivariate normal distribution
- Estimation of the covariance matrix

$$\widehat{\mathbf{V}}_N \quad = \quad \operatorname{diag}\left(\frac{N}{n_i}\widehat{\mathbf{\Sigma}}_i : 1 \leq i \leq a\right),$$

$$\widehat{\mathbf{\Sigma}}_i \quad = \quad \frac{1}{n_i - 1}\sum_{k=1}^{n_i}(\mathbf{X}_{ik} - \overline{\mathbf{X}}_{i\cdot})(\mathbf{X}_{ik} - \overline{\mathbf{X}}_{i\cdot})'.$$

Test Statistics

- Wald-type statistic

$$Q_N(\mathbf{T}) = N \cdot \overline{\mathbf{X}}_{\cdot}' \mathbf{T}(\mathbf{T}\widehat{\mathbf{V}}_N\mathbf{T})^{+}\mathbf{T}\overline{\mathbf{X}}_{\cdot} \sim \chi^2_{rank(\mathbf{T})}, N \to \infty.$$

  - Statistic is not numerically intensive
  - "easy" to compute with standard software
  - Can be used to test general hypotheses in general MANOVA
  - However, very large sample sizes are needed
- Idea: Explore resampling techniques as an approximation for small samples

Nonparametric Bootstrap Test

- Idea: estimate $\chi^2_{1-\alpha}(rank(\mathbf{T}))$ via resampling
- Data: $\mathbf{X} = (\mathbf{X}_{11}', \ldots, \mathbf{X}_{an_a}')'$
  - Draw with replacement from all data: $\mathbf{X}^* = (\mathbf{X}_{11}'^*, \ldots, \mathbf{X}_{an_a}'^*)'$
  - $\mathbf{X}_{11}'^*, , \ldots, \mathbf{X}_{1n_1}'^*$: group 1
  - $\mathbf{X}_{21}'^*, \ldots, \mathbf{X}_{2n_2}'^*$: group 2
  - ...
- Means: $\overline{\mathbf{X}}_{i\cdot}^* = \frac{1}{n_i}\sum_{k=1}^{n_i} \mathbf{X}_{ik}^* \Rightarrow \overline{\mathbf{X}}_{\cdot}^* = (\overline{\mathbf{X}}_{1\cdot}'^*, \ldots, \overline{\mathbf{X}}_{a\cdot}'^*)'$
- Estimated covariance matrix

$$\widehat{\mathbf{V}}_N^* = \operatorname{diag}\Big(\frac{N}{n_i}\widehat{\mathbf{\Sigma}}_i^* : 1 \leq i \leq a\Big),$$

$$\widehat{\mathbf{\Sigma}}_i^* = \frac{1}{n_i - 1}\sum_{k=1}^{n_i}(\mathbf{X}_{ik}^* - \overline{\mathbf{X}}_{i\cdot}^*)(\mathbf{X}_{ik}^* - \overline{\mathbf{X}}_{i\cdot}^*)'.$$

- $Q_N^*(\mathbf{T}) = N \cdot (\overline{\mathbf{X}}_{\cdot}^*)'\mathbf{T}(\mathbf{T}\widehat{\mathbf{V}}_N^*\mathbf{T})^+\mathbf{T}\overline{\mathbf{X}}_{\cdot}^*.$
- Repeat these steps *nboot*-times

Why do Bootstrap Tests work?

- Data $\mathbf{X} = (\underbrace{\mathbf{X}_{11}', \ldots, \mathbf{X}_{1n_1}'}_{\sim F_1}, \underbrace{\mathbf{X}_{21}', \ldots, \mathbf{X}_{2n_2}'}_{\sim \mathbf{F}_2})'$
- Resampling $\mathbf{X}^* = (\underbrace{\mathbf{X}_{11}^{*'}, \ldots, \mathbf{X}_{1n_1}^{*'}}_{\sim \kappa_1 \mathbf{F}_1 + \kappa_2 \mathbf{F}_2}, \underbrace{\mathbf{X}_{21}^{*'}, \ldots, \mathbf{X}_{2n_2}^{*'}}_{\sim \kappa_1 \mathbf{F}_1 + \kappa_2 \mathbf{F}_2})'$
  - $E(E(\overline{X}_{1\cdot}^* - \overline{X}_{2\cdot}^* | \mathbf{X})) = 0$
  - $Var(\sqrt{N}(\overline{X}_{1\cdot}^* - \overline{X}_{2\cdot}^*) | \mathbf{X}) \to \widetilde{\sigma}^2 = \sum_{i=1}^2 \kappa_i \sigma_i^2 + \sum_{i=1}^2 \kappa_i (\mu_i - \sum_{\ell=1}^2 \kappa_\ell \mu_\ell)^2$
  - Variance of resampled means depends on σ_i^2 and μ_i
- Studentization
  - **Consistent estimator of $\widetilde{\sigma}^2$!**

When do Bootstrap Tests Work?

- Distribution of $Q_N^*(\mathbf{T})$ given $\mathbf{X}$
  - Expectation of resampled mean difference: 0
  - Variance of studentized mean: 1
  - $Q_N^*(\mathbf{T})$ is conditionally $\chi^2_{rank(\mathbf{T})}$ (in probability)

Bootstrap test works iff $Q_N(\mathbf{T}) \stackrel{\mathcal{D}}{\to} \chi^2_{rank(\mathbf{T})}$

- In words
  - Resampling dist. mimicks the distribution of $Q_N(\mathbf{T})$ under H_0
  - The dist. of $Q_N(\mathbf{T})$ departs from the resampling dist. under H_1
- References
  - Janssen (1997, 2005), Janssen and Pauls (2003)
  - Konietschke and Pauly (2012 a, b), Konietschke et al. (2015)

Parametric Bootstrap Test

- Data: $\mathbf{X} = (\mathbf{X}'_{11}, \ldots, \mathbf{X}'_{an_a})'$
  - Obtain: $\widehat{\boldsymbol{\Sigma}}_i$
  - $\mathbf{X}'^{*}_{11}, , \ldots, \mathbf{X}'^{*}_{1n_1} \sim N(\mathbf{0}, \widehat{\boldsymbol{\Sigma}}_1)$: group 1
  - $\mathbf{X}'^{*}_{21}, \ldots, \mathbf{X}'^{*}_{2n_2} \sim N(\mathbf{0}, \widehat{\boldsymbol{\Sigma}}_2)$: group 2
  - ...
- Means: $\overline{\mathbf{X}}^{*}_{i\cdot} = \frac{1}{n_i}\sum_{k=1}^{n_i} \mathbf{X}^{*}_{ik} \Rightarrow \overline{\mathbf{X}}^{*}_{\cdot} = (\overline{\mathbf{X}}'^{*}_{1\cdot}, \ldots, \overline{\mathbf{X}}'^{*}_{a\cdot})'$
- Estimated covariance matrix

$$\begin{aligned} \widehat{\mathbf{V}}^{*}_N &= \operatorname{diag}\left(\frac{N}{n_i}\widehat{\boldsymbol{\Sigma}}^{*}_i : 1 \leq i \leq a\right), \\ \widehat{\boldsymbol{\Sigma}}^{*}_i &= \frac{1}{n_i - 1}\sum_{k=1}^{n_i}(\mathbf{X}^{*}_{ik} - \overline{\mathbf{X}}^{*}_{i\cdot})(\mathbf{X}^{*}_{ik} - \overline{\mathbf{X}}^{*}_{i\cdot})'. \end{aligned}$$

- $Q^{*}_N(\mathbf{T}) = N \cdot (\overline{\mathbf{X}}^{*}_{\cdot})'\mathbf{T}(\mathbf{T}\widehat{\mathbf{V}}^{*}_N\mathbf{T})^{+}\mathbf{T}\overline{\mathbf{X}}^{*}_{\cdot}.$
- Repeat these steps *nboot*-times

Simulation Settings - I

- $a = 2, p = 4,\ nsim = nboot = 10,000$

$$
\begin{aligned}
\text{Setting 1: } \boldsymbol{\Sigma}_1 &= \mathbf{I}_4 + 0.5(\mathbf{J}_4 - \mathbf{I}_4) = \boldsymbol{\Sigma}_2 \\
\text{Setting 2: } \boldsymbol{\Sigma}_1 &= [\sigma_{rs}] = (0.6)^{|r-s|} = \boldsymbol{\Sigma}_2 \\
\text{Setting 3: } \boldsymbol{\Sigma}_1 &= \mathbf{I}_4 + 0.5(\mathbf{J}_4 - \mathbf{I}_4) \ \text{ and } \ \boldsymbol{\Sigma}_2 = \mathbf{I}_4 \cdot 3 + 0.5(\mathbf{J}_4 - \mathbf{I}_4) \\
\text{Setting 4: } \boldsymbol{\Sigma}_1 &= [\sigma_{rs}] = (0.6)^{|r-s|} \ \text{ and } \ \boldsymbol{\Sigma}_2 = (0.6)^{|r-s|} + \mathbf{I}_4 \cdot 2
\end{aligned}
$$

Simulation Results - I

		Setting 1				Setting 2				Setting 3				Setting 4			
Dist	(n_1, n_2)	Wald	NB	PB	Wilks	Wald	NB	PB	Wilks	Wald	NB	PB	Wilks	Wald	NB	PB	Wilks
Nor	(10,10)	15.1	5.4	4.8	4.7	14.8	5.2	4.6	4.5	18.3	7.8	5.3	7.3	17.7	7.4	5.0	6.7
	(10,20)	13.4	4.4	5.1	4.8	13.8	4.8	5.5	5.0	11.1	3.3	4.7	1.3	10.7	3.0	4.3	1.1
	(20,10)	13.7	4.7	5.3	5.3	13.8	4.2	4.8	5.1	21.0	10.6	6.8	19.1	20.4	10.1	6.4	19.3
	(20,20)	8.7	4.5	4.4	4.8	8.9	4.9	4.8	5.1	10.2	5.5	4.6	6.8	10.9	6.7	5.4	6.1
T_7	(10,10)	14.9	4.9	4.1	4.8	14.0	4.5	3.8	5.0	18.6	6.8	4.5	6.0	16.8	6.6	4.3	6.3
	(10,20)	13.8	4.3	4.8	4.3	13.9	4.9	5.4	4.9	10.4	3.3	4.7	1.5	9.8	3.0	4.2	1.1
	(20,10)	13.2	3.9	4.3	4.6	13.3	4.3	4.8	4.4	19.5	9.3	5.6	17.9	20.5	9.8	6.3	18.6
	(20,20)	9.0	5.1	4.9	4.6	8.8	4.8	4.6	4.4	10.5	6.3	4.8	5.8	10.6	6.2	4.8	5.6
DE	(10,10)	14.8	4.9	3.4	3.7	14.2	4.8	3.6	4.1	17.7	7.0	4.2	5.6	17.0	6.7	3.9	6.3
	(10,20)	12.9	4.2	4.5	5.2	12.5	5.0	5.2	4.4	10.5	3.2	4.3	1.1	10.2	3.1	4.2	1.1
	(20,10)	12.8	4.2	4.4	5.4	13.9	5.2	5.4	5.1	18.6	9.1	4.8	17.3	18.9	9.2	5.3	17.4
	(20,20)	8.6	5.1	4.4	4.7	8.7	4.9	4.4	4.4	10.0	6.0	4.6	5.8	10.3	6.5	4.8	5.6
χ^2_{15}	(10,10)	15.1	5.0	4.3	4.8	14.4	4.8	4.1	4.5	18.4	8.1	5.4	7.1	19.0	7.8	5.2	7.3
	(10,20)	14.2	4.6	5.5	5.1	13.7	4.6	5.3	5.1	11.4	3.1	4.6	1.4	10.5	3.3	4.6	1.5
	(20,10)	13.1	4.2	4.9	4.7	13.6	4.7	5.6	5.1	21.6	10.3	6.7	19.1	21.2	10.5	6.9	18.7
	(20,20)	9.3	5.1	4.8	4.5	8.1	4.8	4.7	4.7	10.7	6.3	5.1	6.3	10.7	6.9	5.6	6.5
χ^2_{20}	(10,10)	15.2	5.2	4.5	4.6	14.1	5.0	4.4	5.4	18.5	8.1	5.6	7.3	19.9	9.1	6.3	7.2
	(10,20)	13.9	4.9	5.6	5.2	13.4	4.5	5.2	4.5	10.8	3.3	4.8	1.3	10.6	3.2	4.8	1.3
	(20,10)	14.1	4.4	5.1	5.1	13.7	4.6	5.4	4.8	21.5	11.1	7.0	18.3	21.8	10.4	6.9	18.8
	(20,20)	9.1	5.3	5.0	4.1	8.6	5.0	4.8	5.0	10.5	6.3	5.0	6.3	12.6	7.7	6.2	6.7

Simulation Settings - II

- $a = 4, p = 4,\ nsim = nboot = 10,000$

$$
\begin{aligned}
\text{Setting 5: } \boldsymbol{\Sigma}_i &= \mathbf{I}_4 + 0.5(\mathbf{J}_4 - \mathbf{I}_4), i = 1, \ldots, 4, \\
\text{Setting 6: } \boldsymbol{\Sigma}_i &= [\sigma_{i,rs}] = (0.6)^{|r-s|}, i = 1, \ldots, 4, \\
\text{Setting 7: } \boldsymbol{\Sigma}_i &= \mathbf{I}_4 \cdot i + 0.5(\mathbf{J}_4 - \mathbf{I}_4), i = 1, \ldots, 4, \\
\text{Setting 8: } \boldsymbol{\Sigma}_i &= [\sigma_{i,rs}] = (0.6)^{|r-s|} + \mathbf{I}_4 \cdot i, i = 1, \ldots, 4,
\end{aligned}
$$

Simulation Results - II

Dist	n	Setting 5 Wald	NB	PB	Wilks	Setting 6 Wald	NB	PB	Wilks	Setting 7 Wald	NB	PB	Wilks	Setting 8 Wald	NB	PB	Wilks
Nor	n_5	37.1	3.7	4.4	4.8	35.0	3.9	5.1	4.8	39.8	5.1	4.9	5.0	39.8	4.9	4.9	5.3
	n_6	15.9	4.2	4.7	4.8	17.8	5.2	5.8	5.3	17.5	5.5	5.0	5.7	18.2	5.0	4.5	5.5
	n_7	38.8	3.4	5.4	4.9	38.4	4.8	6.4	5.3	34.1	2.2	5.2	2.4	33.3	2.2	4.8	2.8
	n_8	38.1	3.6	5.4	4.7	40.4	3.4	5.2	4.9	48.4	9.2	7.3	9.6	47.4	11.7	8.6	9.9
T_7	n_5	36.0	3.9	4.6	4.7	36.2	4.7	5.1	4.6	37.7	4.9	4.5	4.9	38.5	4.4	3.8	4.7
	n_6	16.0	4.4	4.6	4.7	15.9	5.3	5.2	5.4	17.6	6.0	5.3	5.3	16.9	5.5	5.2	4.8
	n_7	38.5	3.5	5.1	5.1	41.1	4.7	6.6	4.9	30.8	1.8	3.9	2.7	32.9	1.9	4.9	2.5
	n_8	38.3	3.7	5.6	5.1	39.7	4.1	5.4	5.3	45.3	8.1	6.4	9.8	48.4	9.4	7.0	9.7
DE	n_5	35.1	3.1	3.3	4.5	36.0	2.6	2.6	4.5	37.4	4.0	3.2	4.3	37.9	3.5	2.9	4.4
	n_6	15.9	4.5	4.3	4.6	15.4	4.6	4.1	4.8	16.3	4.8	4.0	4.6	15.6	3.6	3.1	4.6
	n_7	36.7	3.3	4.1	4.6	36.5	3.1	4.5	5.0	31.4	2.3	3.7	2.2	30.5	1.9	3.8	2.1
	n_8	37.1	3.6	4.4	5.2	35.4	3.3	3.3	4.8	45.5	8.3	5.6	9.0	4.2	6.5	4.0	9.3
χ^2_{15}	n_5	37.6	3.6	4.9	5.3	38.1	3.9	4.7	4.7	40.5	5.4	5.2	5.2	40.9	5.1	4.8	5.7
	n_6	17.2	4.8	5.3	4.4	20.2	4.6	5.2	4.7	19.0	5.7	5.6	5.3	18.7	5.1	4.4	5.6
	n_7	40.3	4.5	6.5	5.3	41.8	4.7	7.6	4.9	35.6	2.6	5.3	2.9	33.6	2.5	4.9	2.7
	n_8	41.1	4.3	6.6	4.7	38.0	4.1	6.1	5.6	49.3	9.9	8.0	10.4	46.9	9.0	6.7	10.6
χ^2_{20}	n_5	37.9	3.6	4.5	5.2	35.0	3.5	4.5	5.2	40.1	5.4	4.9	5.2	38.9	5.2	5.1	4.8
	n_6	15.9	4.6	4.9	4.8	16.8	5.2	5.5	5.1	18.7	5.2	5.1	5.2	18.2	5.4	5.1	4.4
	n_7	38.7	3.5	5.6	5.6	42.0	3.7	6.0	5.6	33.7	2.6	5.4	2.6	33.2	3.0	5.0	2.3
	n_8	39.5	4.0	6.2	5.2	38.9	4.0	5.8	5.2	4.7	9.5	7.8	10.5	49.2	9.7	7.0	10.0

Simulation Results

- Procedures seem to be “robust” against non-normality
- Depends on the amount of skewness
- Severe settings: Positive and negative pairings
- Parametric bootstrap is the most accurate procedure
- ... but not always accurate...

Summary

- Resampling methods for General MANOVA
  - Conditional CLT for studentized resampling tests
  - Resampling distributions are invariant under main effects
  - Asymptotic tests
- Repeated measures designs
  - $\mathbf{X}_k = (X_{1k}, X_{2k})'$, $k = 1, \dots, n$, $E(\mathbf{X}_1) = \boldsymbol{\mu}$ and $Cov(\mathbf{X}_1) = \boldsymbol{\Sigma}$
  - Permutation tests für $H_0 : \mu_1 = \mu_2$
    - Permuting all data $\mathbf{X} = (X_{11}, \dots, X_{2n})'$ (K. and Pauly 2012)
  - $\mathbf{X}_k = (X_{1k}, X_{2k}, \dots, X_{dk})'$, $k = 1, \dots, n$
  - $E(\mathbf{X}_1) = \boldsymbol{\mu}$ and $Cov(\mathbf{X}_1) = \boldsymbol{\Sigma}$
  - Permutation tests lor low- and high-dimensional data
  - Multiple comparisons

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