頻度論とベイズをつなぐ統計的信頼度

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最近の様子@下平研

深層クロスドメインマッチング相関分析の提案とその応用
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クロスドメインマッチング相関分析 (CDMCA) [1]
人工データを用いた実験
画像-マルチタグ間の相互検索への応用
提案法：深層クロスドメインマッチング相関分析 (DCDMCA)

D2-17
クロスドメインマッチング相関分析を用いた
単語と画像の同時埋め込み
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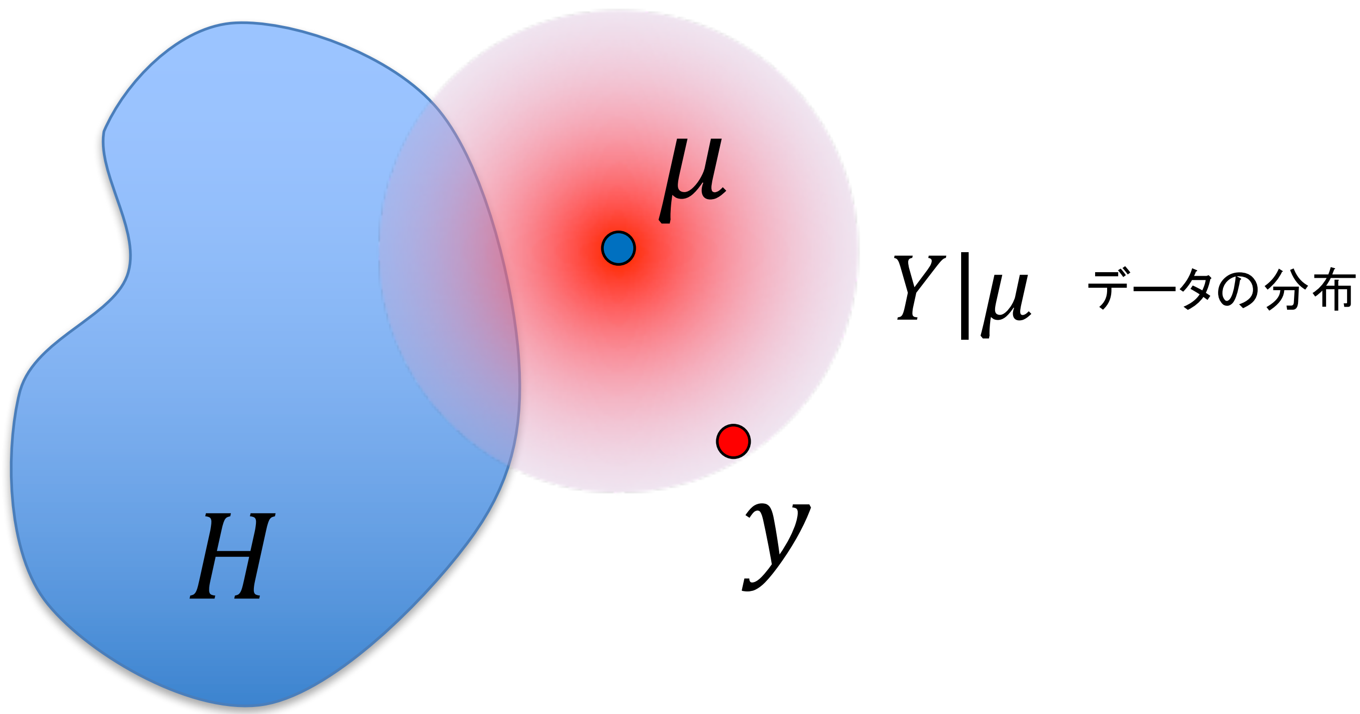
1. はじめに
2. 画像情報を組み合わせた単語埋め込み
2.1 実験1: Word Similarity Task
2.2 実験2: 単語ベクトル, 画像ベクトル間の演算
3. 参考文献

本日のトーク：　地味にやってる話

- Multiple comparisons of log-likelihoods with applications to phylogenetic inference. H Shimodaira, M Hasegawa. *Molecular biology and evolution* 16, 1114-1116, 1999
- An approximately unbiased test of phylogenetic tree selection. H Shimodaira. *Systematic biology* 51 (3), 492-508, 2002
- Approximately unbiased tests of regions using multistep-multiscale bootstrap resampling. H Shimodaira. *The Annals of Statistics* 32, 2004
- Testing regions with nonsmooth boundaries via multiscale bootstrap. H Shimodaira. *Journal of Statistical Planning and Inference* 138, 1227-1241, 2008
- Higher-order accuracy of multiscale-double bootstrap for testing regions. H Shimodaira. *Journal of Multivariate Analysis* 130, 208-223, 2014

マルチスケール・ブートストラップ法による信頼度計算の研究

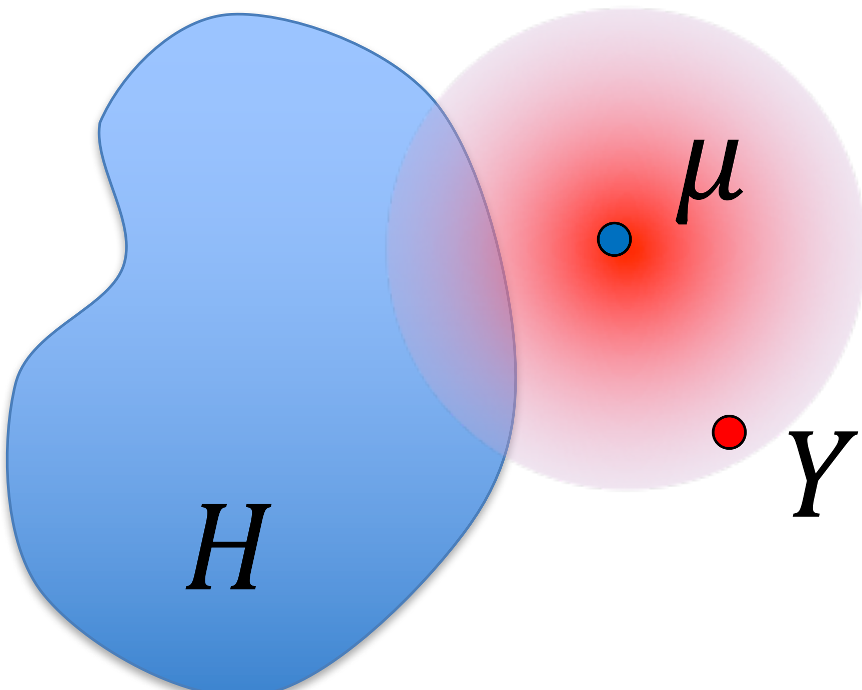
領域の検定と信頼度



$$\mathrm{confidence}(\mu \in H|y)$$

信頼度が小さい時，仮説を棄却する

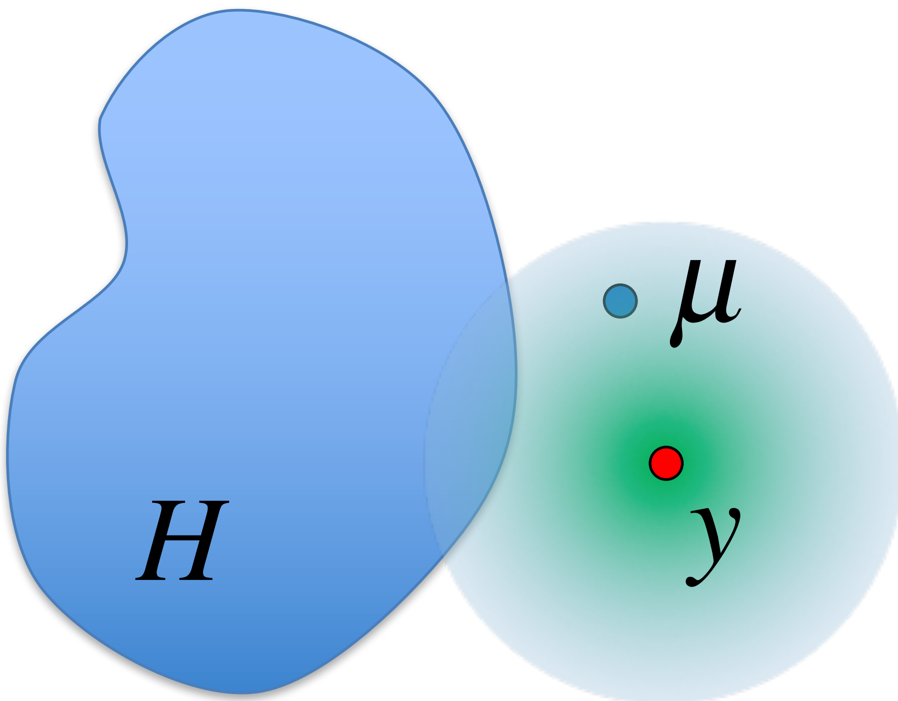
多変量正規モデルで考える



$$Y|\mu \sim N(\mu, I)$$

$$density \propto \exp(-\|y-\mu\|^2/2)$$

ベイズ事後確率は容易に計算



$$Y|\mu \sim N(\mu, I)$$

$$\mu \sim uniform$$

$$density \propto \exp(-\|y-\mu\|^2/2)$$

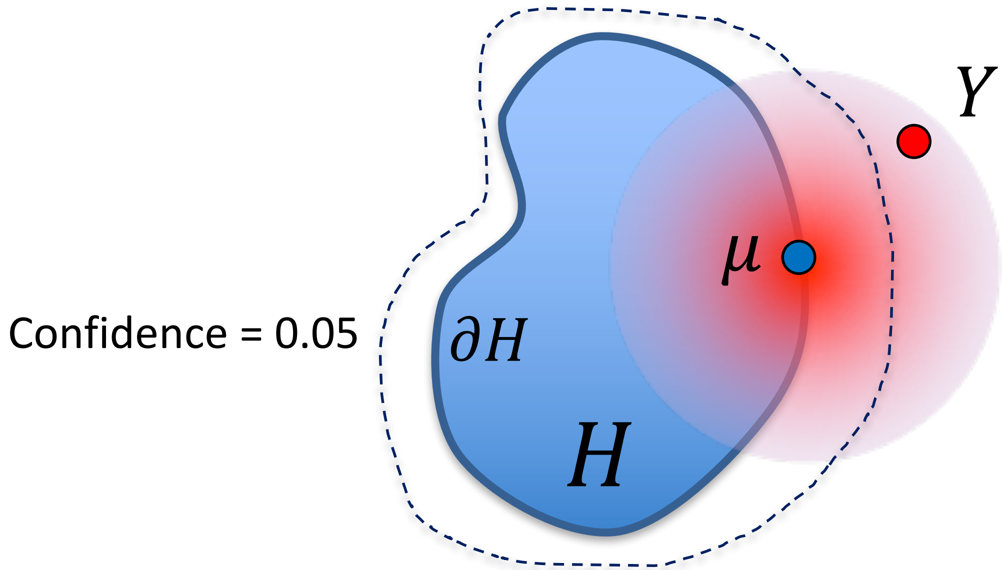
$$\mu \mid y \sim N(y, I)$$

muの事後分布　＝　ブートストラップ分布

$$\mathrm{confidence}_{Bayes}(\mu \in H|y) = P(\mu \in H|y)$$

Hの事後確率　＝　ブートストラップ確率

頻度論のp-値が満たすべき性質



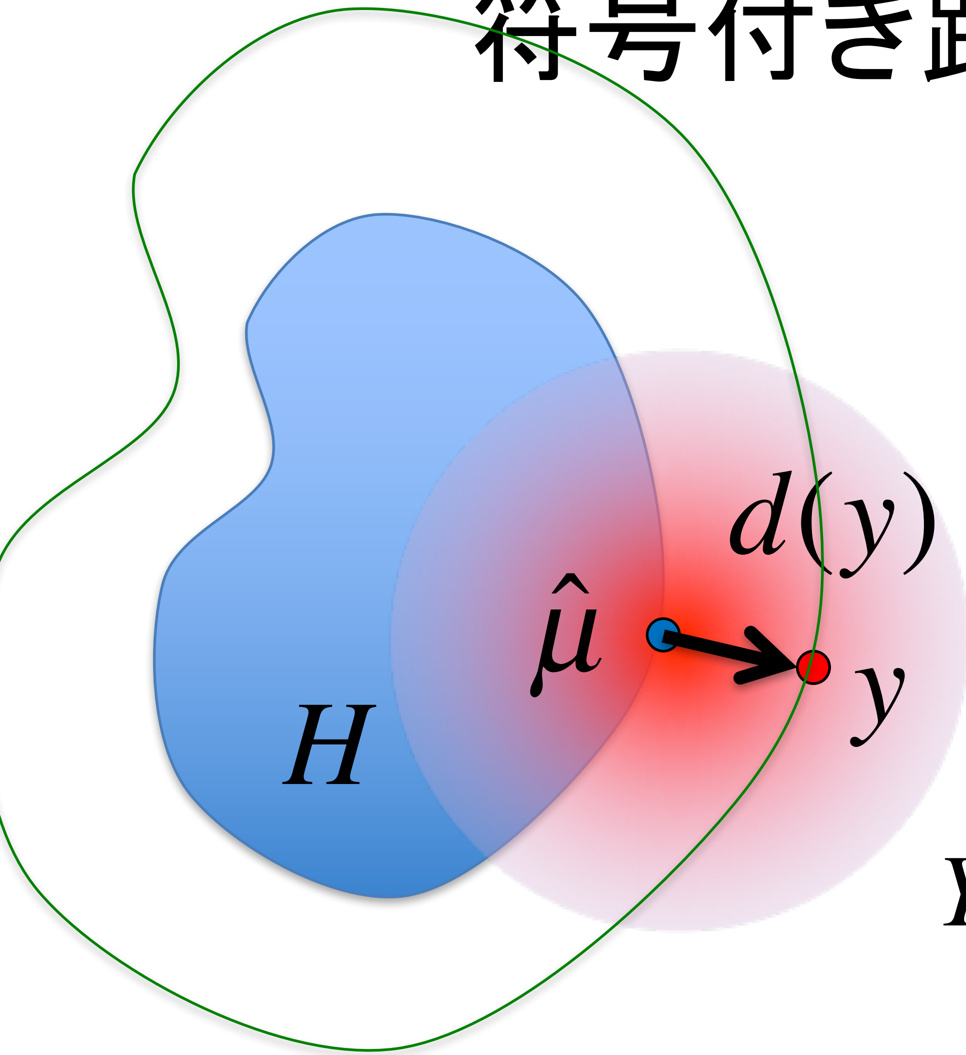
Type-I errorを有意水準(=0.05)で抑えたい．しかし検出力を上げるには等号に近い方が良い．

$$P[\mathrm{confidence}_{freq}(\mu \in H|Y) < 0.05] \leq 0.05 \text{ under } \underline{\mu \in H}$$

不偏検定では，仮説境界上でType-I errorを有意水準と同じにしたい

$$P[\mathrm{confidence}_{freq}(\mu \in H|Y) < 0.05] = 0.05 \text{ under } \underline{\mu \in \partial H}$$

符号付き距離を使う



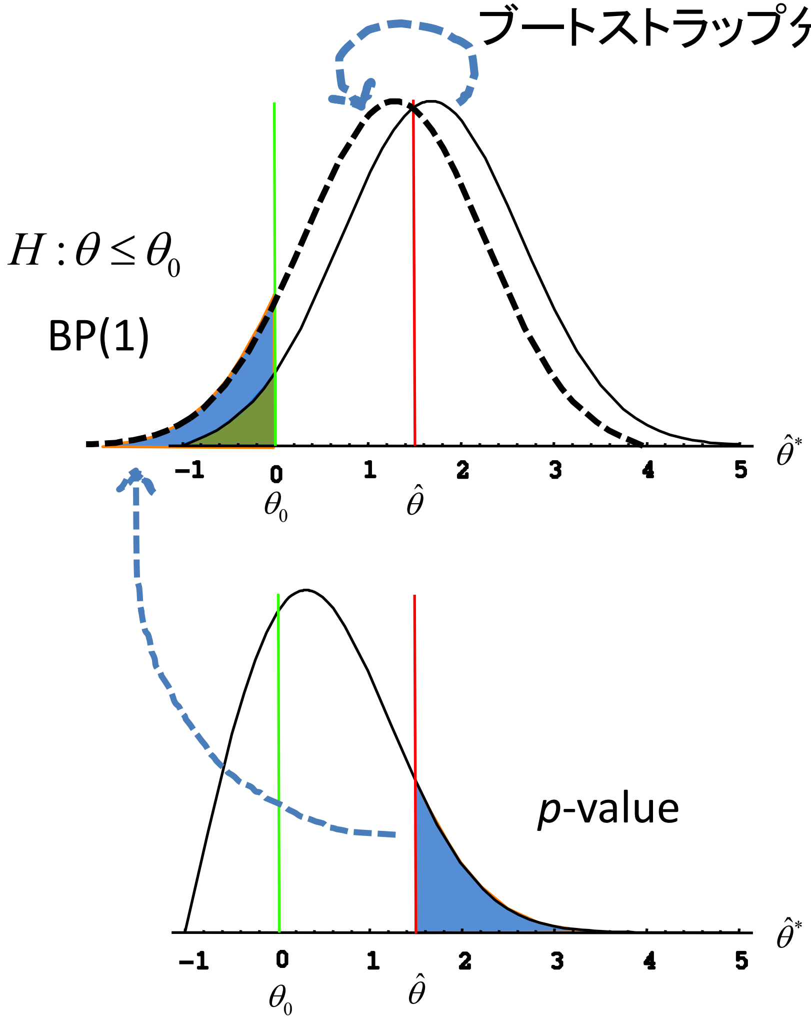
符号付き距離
(signed distance)

$$Y \mid y \sim N(\hat{\mu}, I)$$

$$\text{confidence}_{freq}(\mu \in H|y) = P(d(Y) > d(y)|\hat{\mu}) + O_p(n^{-\frac{3}{2}})$$

もしパラメータにアクセスすれば簡単

ブートストラップ分布をひっくり返す



データからブートストラップ分布

帰無仮説からシミュレーション

ベイズ事後確率はp-値を近似する

多変量正規モデル，平坦な事前分布，仮説領域の境界が滑らかであることを仮定すると

$$\text{confidence}_{freq}(\mu \in H|Y) = \text{confidence}_{Bayes}(\mu \in H|Y) + O_p(n^{-\frac{1}{2}})$$

たしかに近似してるけど，誤差が大きい．誤差の主な原因は，仮説境界の「平均曲率」．

頻度論の意味でp-値を追求してみる．

ブートストラップ法で計算したい．カウント値だけをつかう．

多重比較との関連．

たとえば、モデル選択

- 多項式回帰モデルの次数選択
- 適切なモデルをAIC最小化法で選ぶ

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon$$

各領域がモデルに相当

多項式回帰の次数選択：　次数＝０，１，２から選ぶ

1688　　B. EFRON AND R. TIBSHIRANI

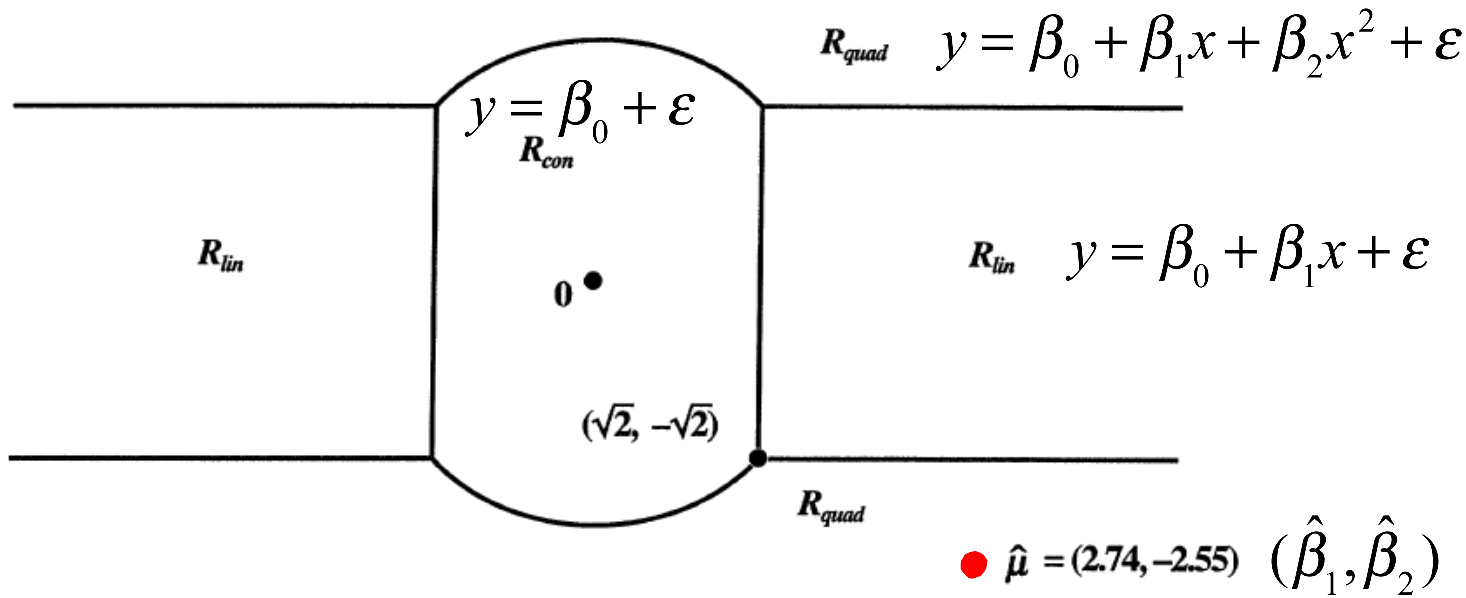


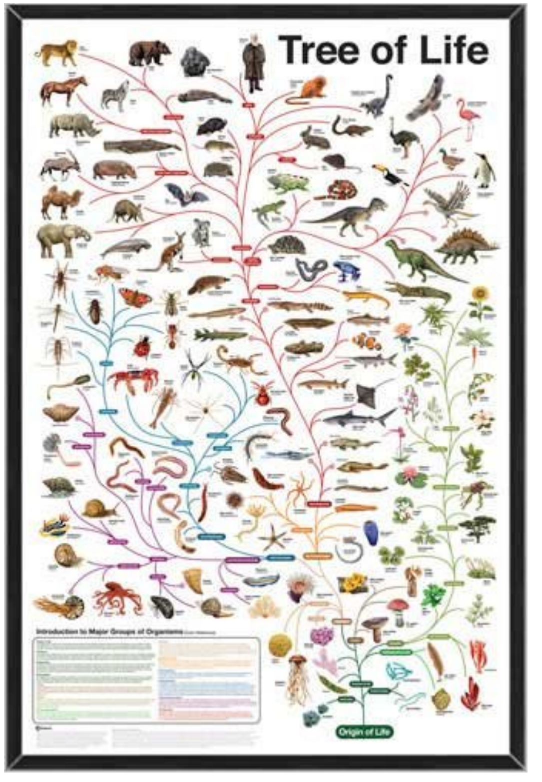
FIG. 1. *An example of the problem of regions: a normally distributed vector $y=\hat{u}$, with covariance I, is observed to lie in the region $\mathscr{R}_{\text{quad}}$. With what confidence can we say that the true expectation vector μ lies in $\mathscr{R}_{\text{quad}}$? This example, which concerns the choice of a polynomial regression model using the C_p criterion, is discussed in Section 5.*

Efron and Tibshirani (1998)　　“The problem of regions”

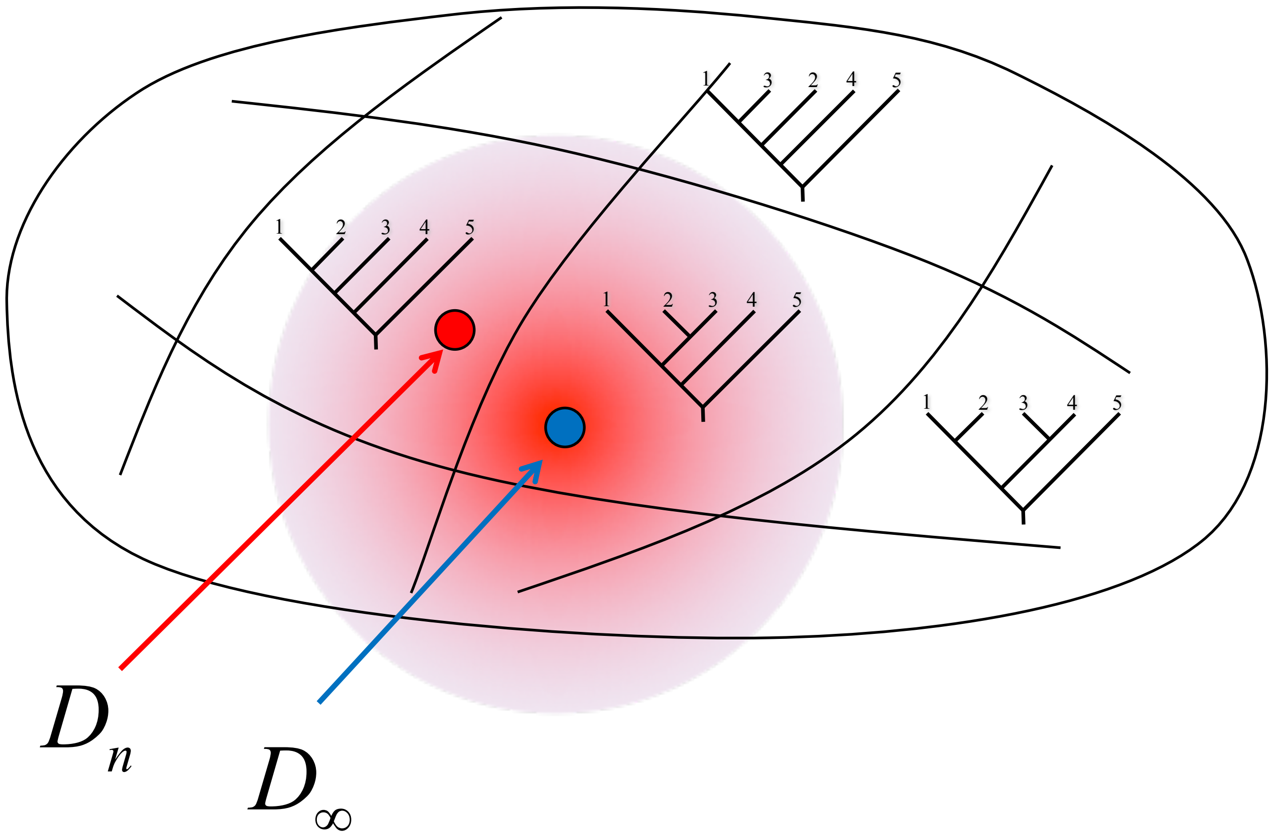
たとえば、進化系統樹の推定

- DNA配列データ
- 系統樹上のマルコフ過程

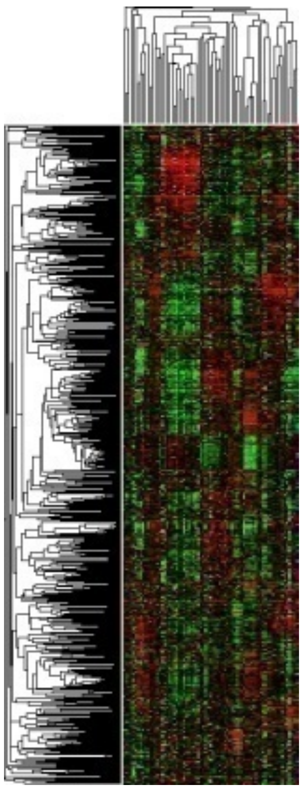
- 最尤法でモデル選択する



各領域が系統樹に相当



Pvclust: Suzuki and Shimodaira (2006)



Pvclust

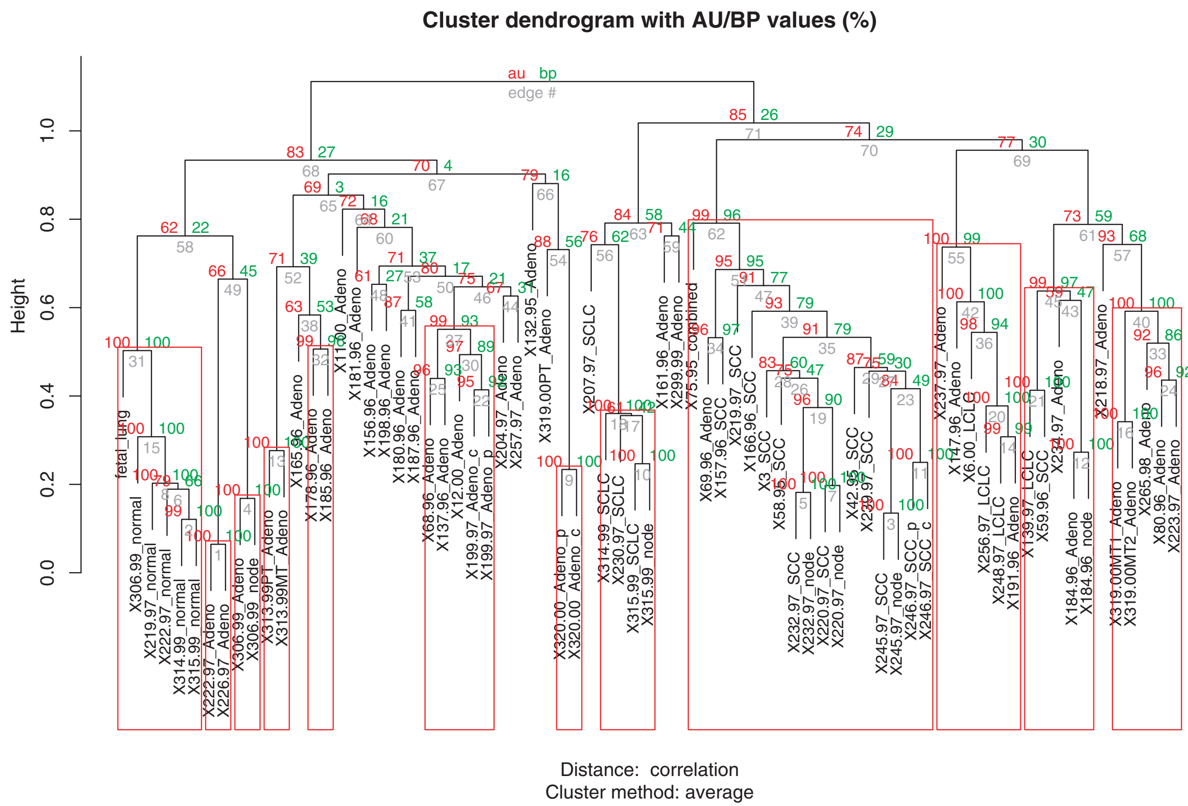


Fig. 1. Hierarchical clustering of 73 lung tumors. The data are expression pattern of 916 genes of Garber *et al.* (2001). Values at branches are AU *p*-values (left), BP values (right), and cluster labels (bottom). Clusters with AU $\geq$ 95 are indicated by the rectangles. The fourth rectangle from the right is a cluster labeled 62 with AU = 0.99 and BP = 0.96.

LETTER

doi:10.1038/nature12969

Bidirectional developmental potential in reprogrammed cells with acquired pluripotency

Haruko Obokata[1,2,3], Yoshiki Sasai[4], Hitoshi Niwa[5], Mitsutaka Kadota[6], Munazah Andrabi[6], Nozomu Takata[4], Mikiko Tokoro[2], Yukari Terashita[1,2], Shigenobu Yonemura[7], Charles A. Vacanti[3] & Teruhiko Wakayama[2,8]

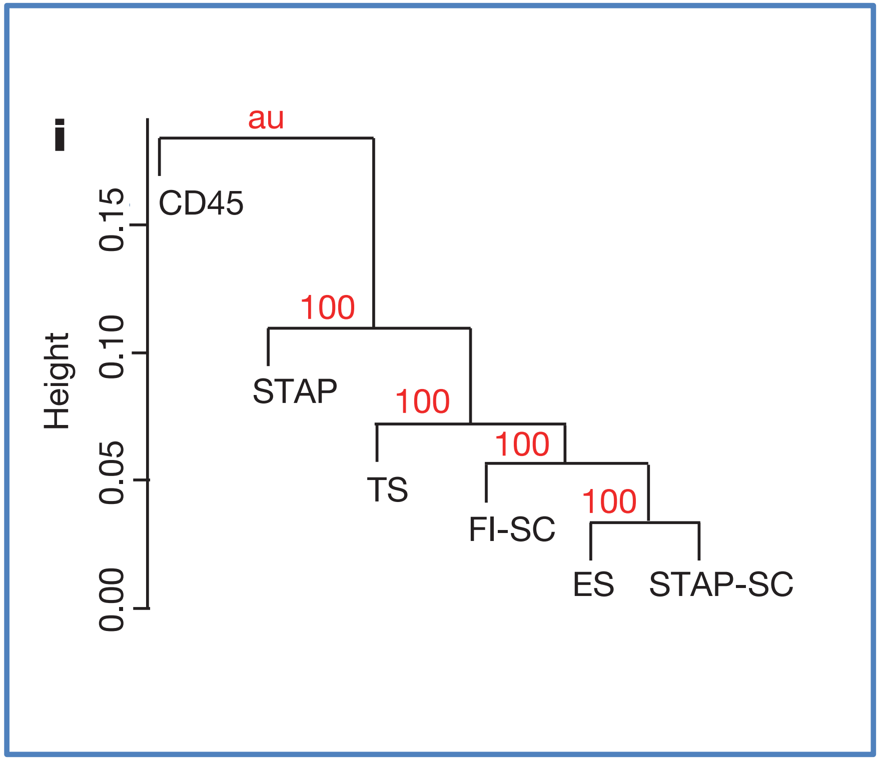
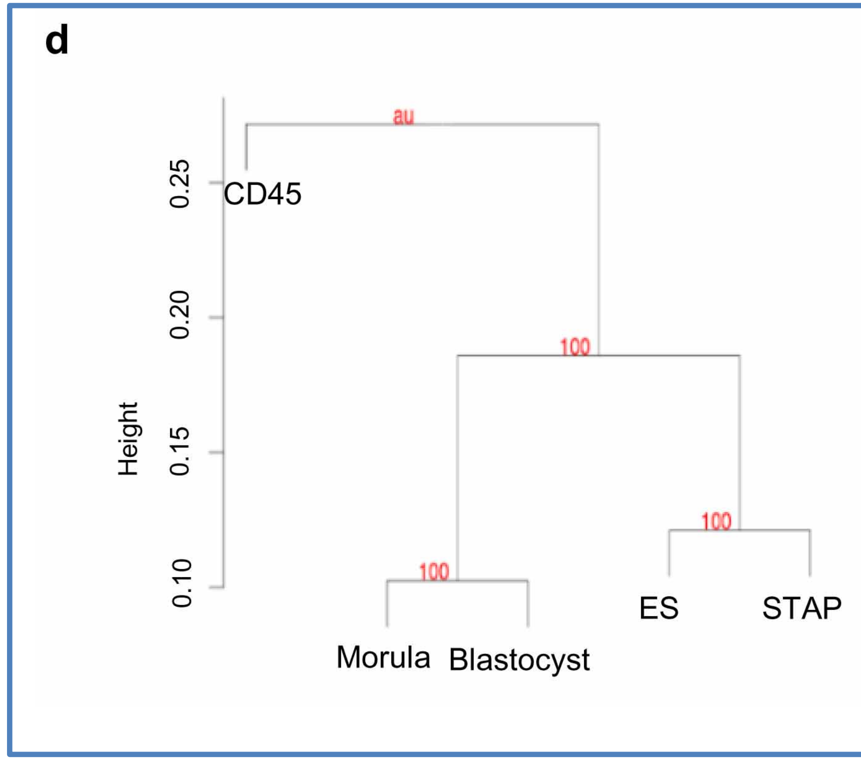


Figure 2 | Fgf4 treatment induces some trophoblast-lineage character in STAP cells.

placental tissues at a detectable level. **i**, Cluster tree diagram from hierarchical clustering of global expression profiles. Red, approximately unbiased *P* values. **j**, qPCR analysis of Fgf4-induced cells



Extended Data Figure 6 | Characterization of ES-like cells converted from Fgf4-induced stem cells and comparison of STAP cells with early embryos.

Scale bar, 100 μm. **d**, Cluster tree diagram from hierarchical clustering of global expression profiles. Red, AU *P* values. As this analysis included morula and blastocyst embryos from which only small amounts of RNA could be obtained, we used pre-amplification with the SMARTer Ultra Low RNA kit for Illumina Sequencing (Clontech Laboratories). **e**, **f**, Volcano plot of the expression

各領域がクラスタに相当

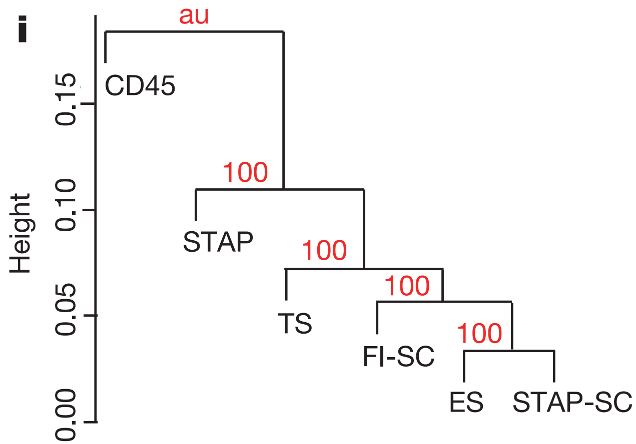
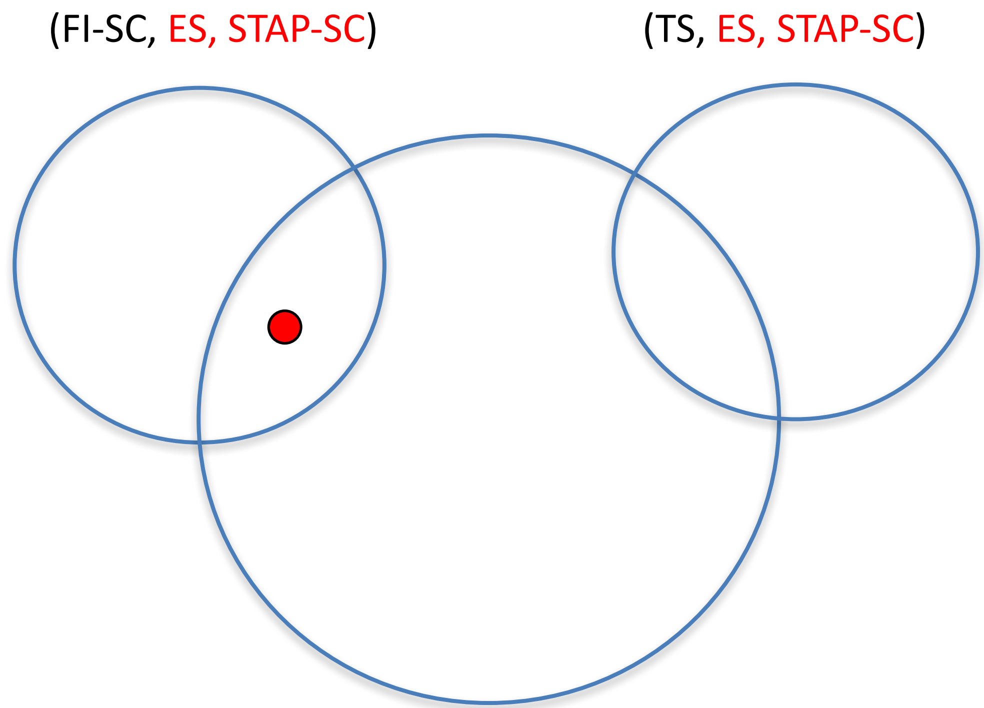
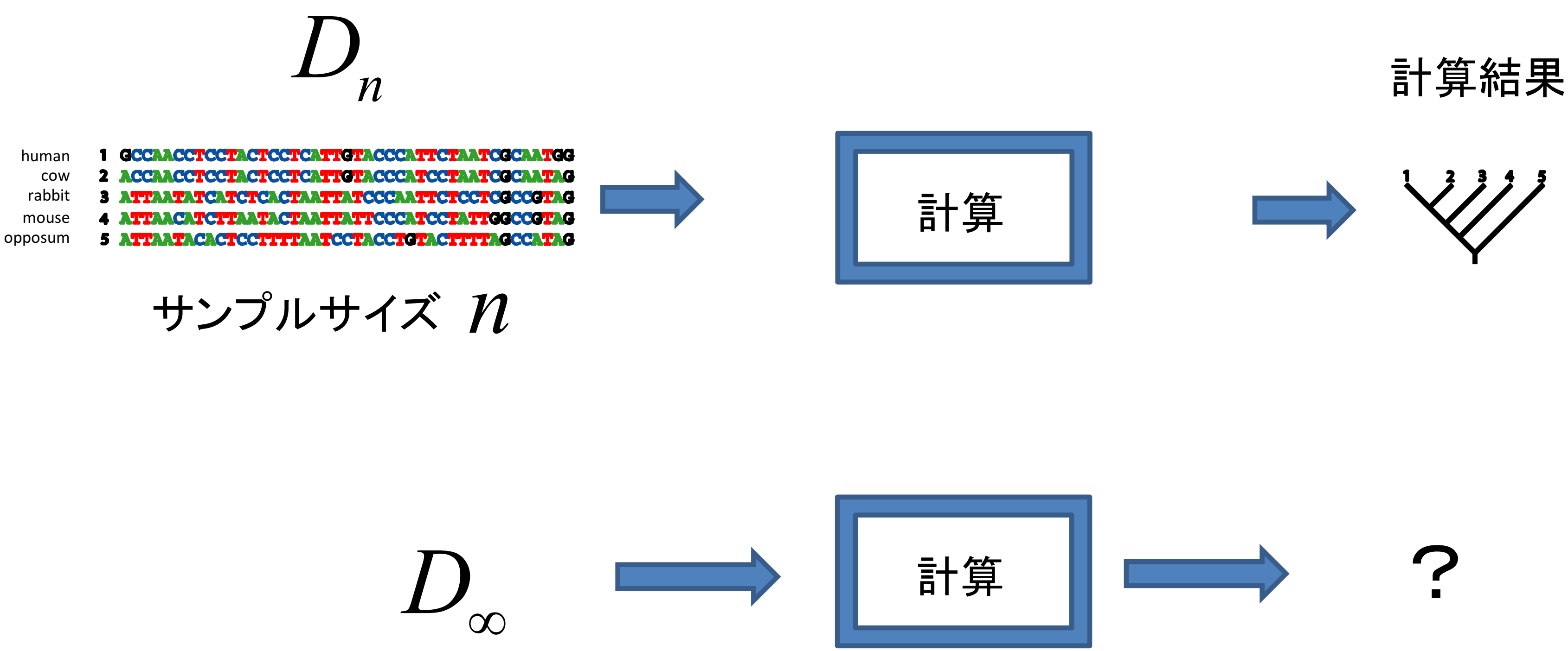


Figure 2 | Fgf4 treatment induces some trophoblast-lineage character in STAP cells.



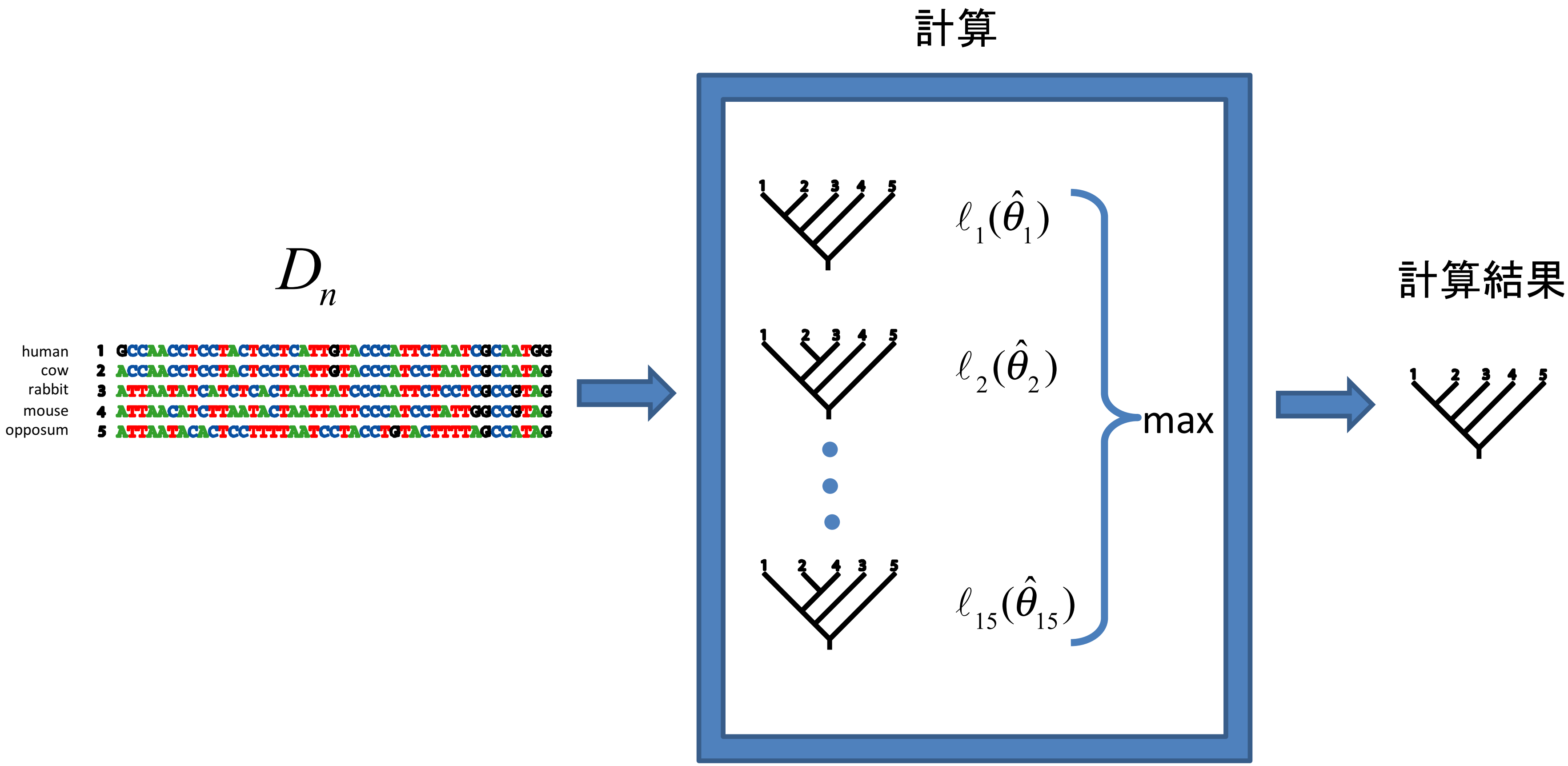
(ES, STAP-SC)がクラスタになる全てのデンドログラムに相当する領域

系統樹の信頼度は？

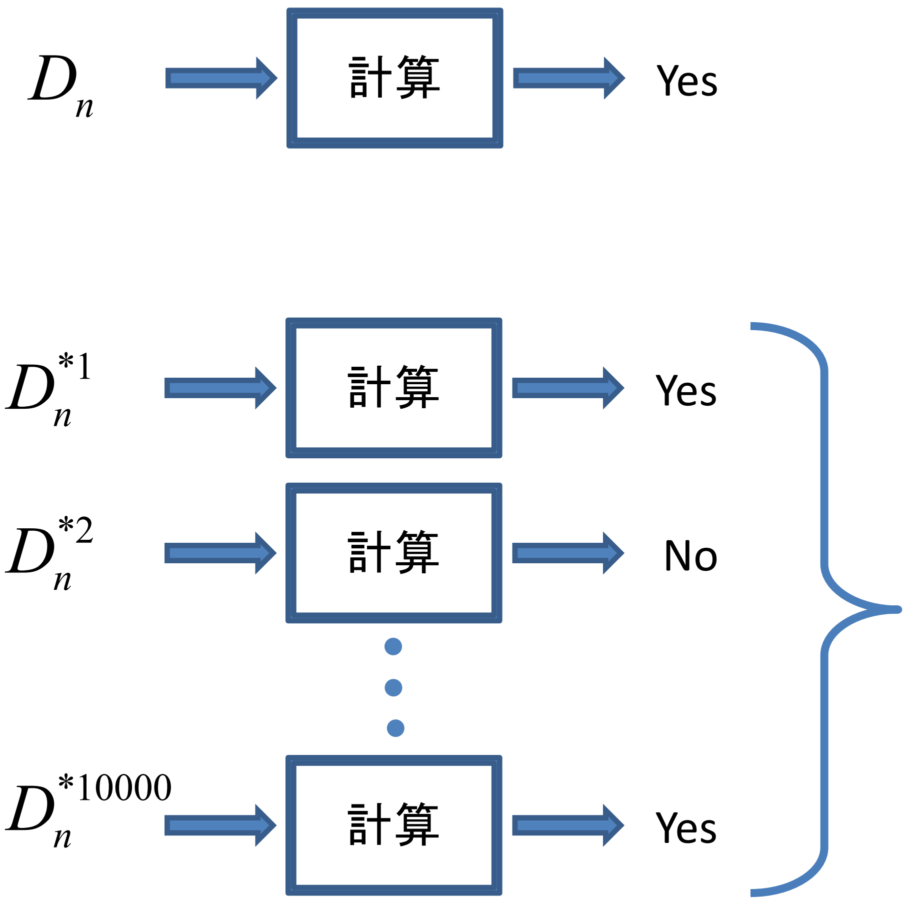


D_n
human 1 GCCAACCTCCTACTCCTCATTGTACCCATTCTAATCGCAATGG
cow 2 ACCAACCTCCTACTCCTCATTGTACCCATCCTAATCGCAATAG
rabbit 3 ATTAATATCATCTCACTAATTATCCCAATTCTCCTCGCCGTAG
mouse 4 ATTAACATCTTAATACTAATTATTCCCATCCTATTGGCCGTAG
opposum 5 ATTAATACACTCCTTTTAATCCTACCTGTACTTTTAGCCATAG
サンプルサイズ n
計算
計算結果
1 2 3 4 5
D_∞
計算
？

「計算」はブラックボックスとみなす



反復計算してカウントだけ使う

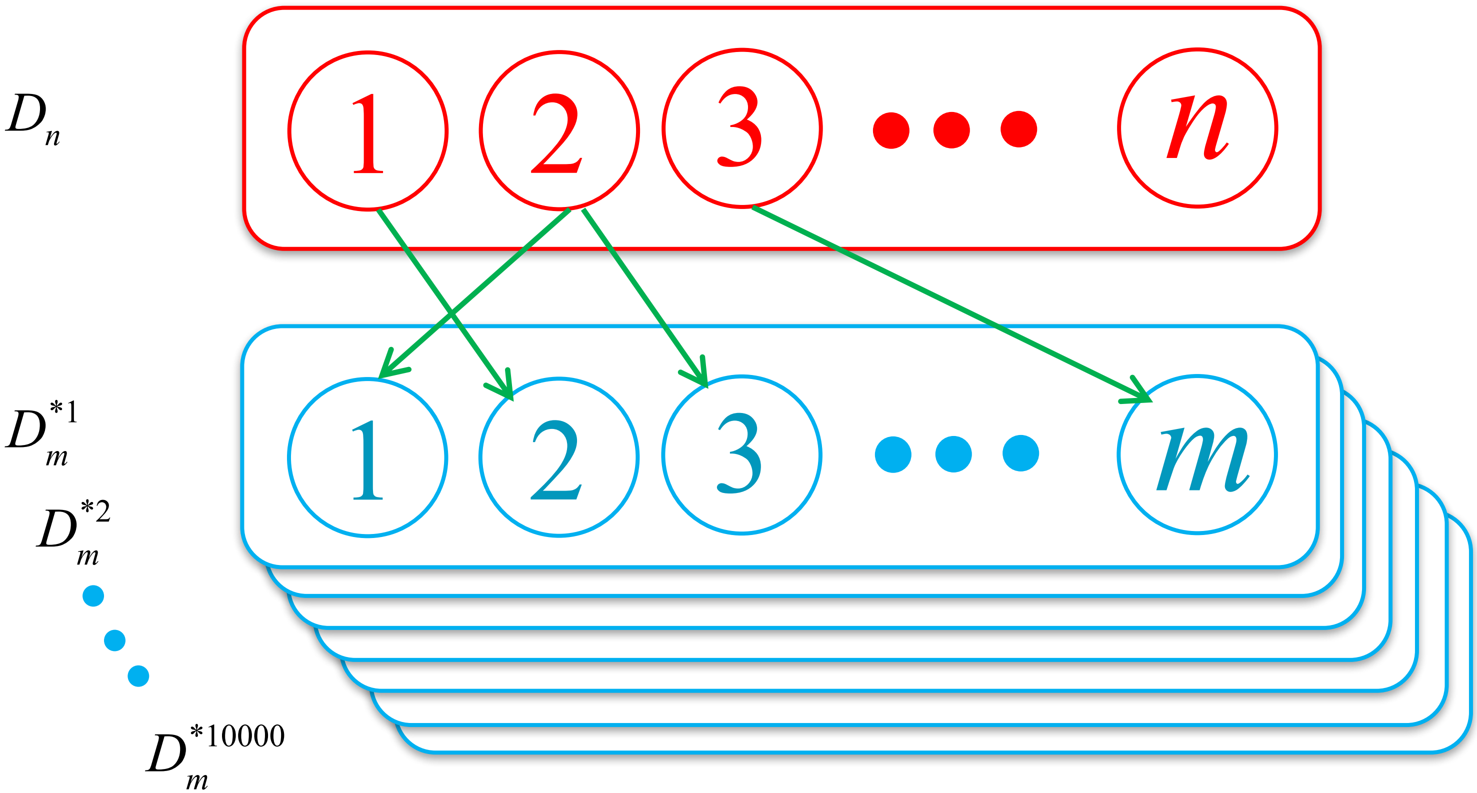


$$\mathrm{BP} = \frac{\#\{Yes\}}{10000} \approx P(Yes \mid Data)$$

Bootstrap Probability

ブートストラップ確率

ランダムに要素をコピーする



ブートストラップ・リサンプリング

Efron (1979)
Felsenstein (1985)

Bootstrap: *n*=10,242 columns

human	1	GCCAACCTCCTACTCCTCATTGTACCCATTCTAATCGCAATGG
cow	2	ACCAACCTCCTACTCCTCATTGTACCCATCCTAATCGCAATAG
rabbit	3	ATTAATATCATCTCACTAATTATCCCAATTCTCCTCGCCGTAG
mouse	4	ATTAACATCTTAATACTAATTATTCCCATCCTATTGGCCGTAG
opposum	5	ATTAATACACTCCTTTTAATCCTACCTGTACTTTTAGCCATAG

Assume i.i.d. for columns

$$D_n \Rightarrow D_m^{*1},\dots,D_m^{*100}$$

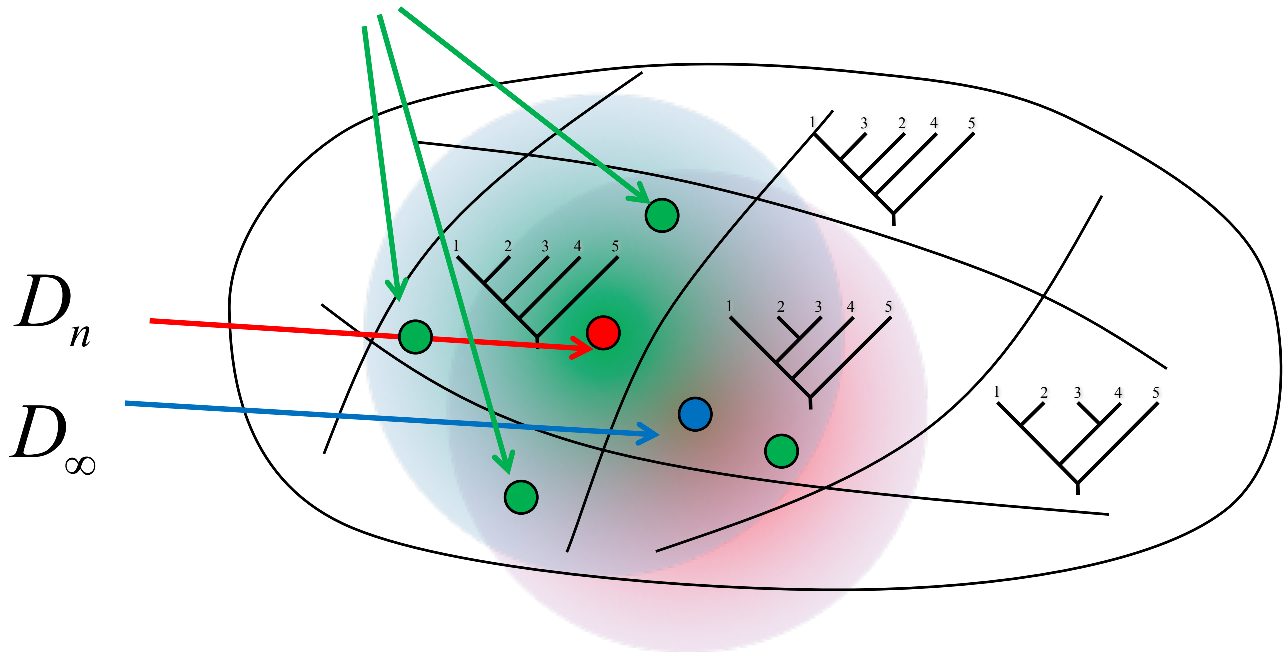
We assume $m = O(n)$, typically m=10242, 5000, 20000, say

In the "*m*-out-of-*n* bootstrap" $0 < m \ll n$, typically m=30, say

BPはベイズ事後確率

Efron and Tibshirani (1998)

$$D_n^{*1}, D_n^{*2}, D_n^{*3}, \ldots \qquad BP = P(Tree \mid data) \approx \frac{\#\{Tree\}}{100}$$



Shimodiara (2002)のマルチスケール・ブートストラップ：D_m^*のバラツキ（分散）はmに反比例する

mを変化させたBPから，各仮説領域までの符号付き距離や，仮説境界の平均曲率がわかる！

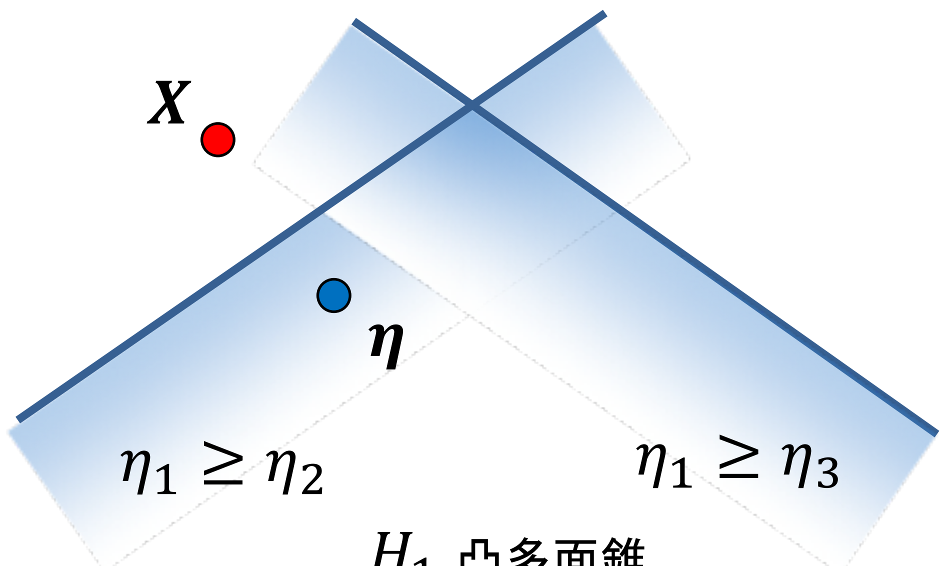
たとえば，多重比較

$\boldsymbol{X} \sim N(\boldsymbol{\eta}, \frac{1}{n}\Sigma)$

H_1: $\eta_1 \geq \eta_2, \ldots, \eta_1 \geq \eta_p$

$$\boldsymbol{X} = \begin{pmatrix} 3.5 \\ 4.0 \\ 0.5 \end{pmatrix}$$

$$\boldsymbol{\eta} = \begin{pmatrix} 3.5 \\ 3.0 \\ 0.5 \end{pmatrix}$$



H_1 凸多面錐

多重比較の場合

$\boldsymbol{X} \sim N(\boldsymbol{\eta}, \frac{1}{n}\Sigma)$

$\boldsymbol{Y} = \sqrt{n}\Sigma^{-1/2}\boldsymbol{X}$
$\boldsymbol{\mu} = \sqrt{n}\Sigma^{-1/2}\boldsymbol{\eta}$

$d_1(Y) = \max\{c_2(X_2 - X_1), \ldots, c_p(X_p - X_1)\}$

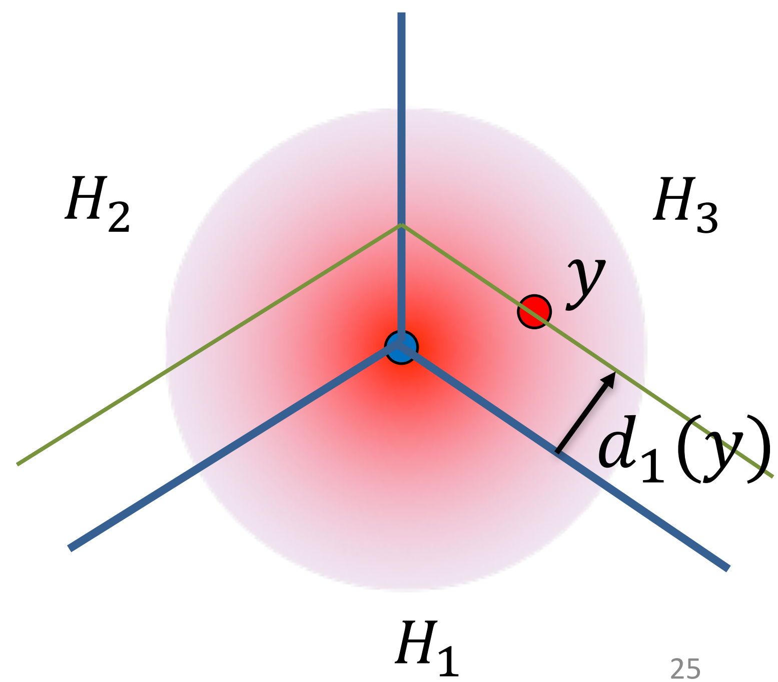
$\boldsymbol{Y} \sim N(\boldsymbol{\mu}, I)$

$$\mathrm{confidence}_{mc}(\mu \in H_1|y) = P(d_1(Y) > d_1(y)|0)$$

Least favorable configuration

$\eta_1 = \eta_2 = \cdots = \eta_p$

仮説領域（凸錘）の頂点



多重比較は保守的

各領域のType-I error

$$P[\mathrm{confidence}_{mc}(\mu \in H_i|y) < 0.05] \leq 0.05 \ \ \text{under } H_i$$

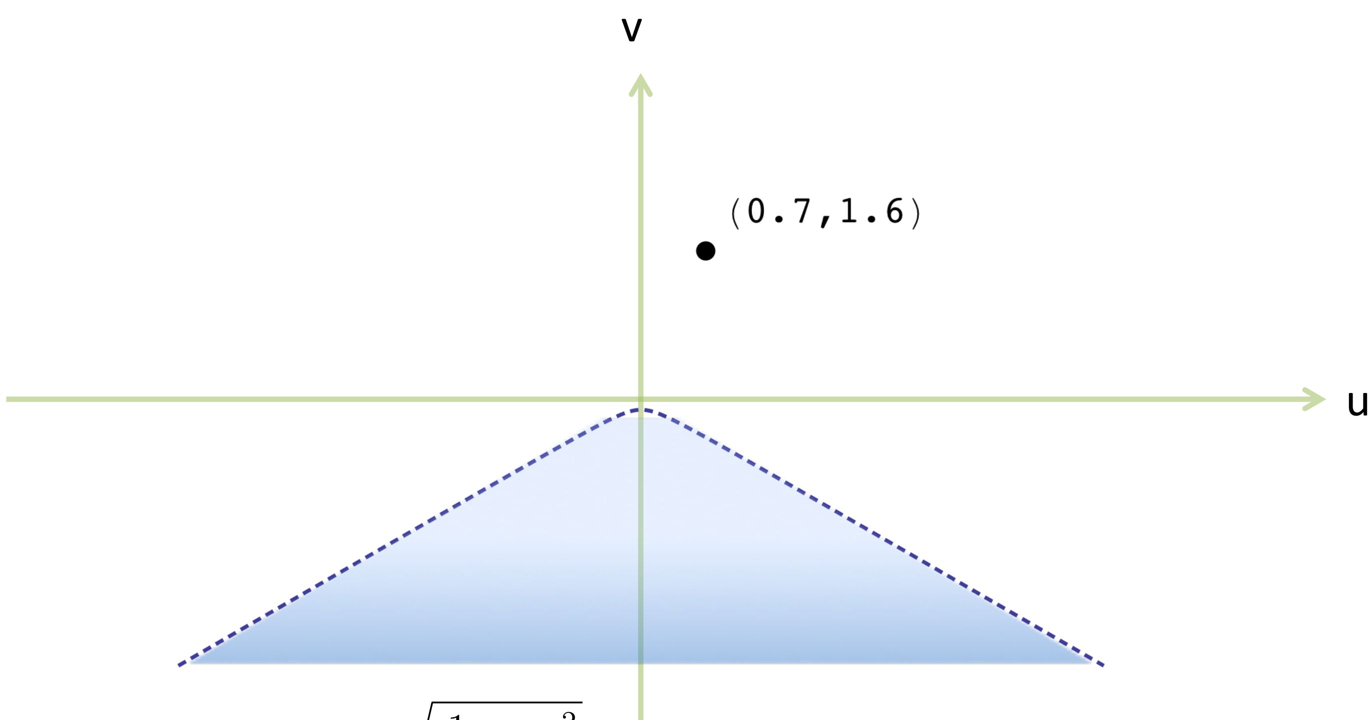
仮説境界上で等号なら嬉しいが，等号になるのはl.f.c.のみ

仮説の信頼集合

$$S(y) = \{H_i\colon \mathrm{confidence}_{mc}(\mu \in H_i|y) \geq 0.05\}$$

$$P[H_i \notin S(y)] \leq 0.05 \ \ \text{under } H_i$$

Region and a data-point



$$v \leq -\sqrt{\frac{1}{64} + \frac{u^2}{3}}$$

Multivariate Normal Model

$$y = (u, v) \in \mathbb{R}^{q+1} \qquad q = \dim u$$

$$Y \sim N_{q+1}(\mu, I_{q+1})$$

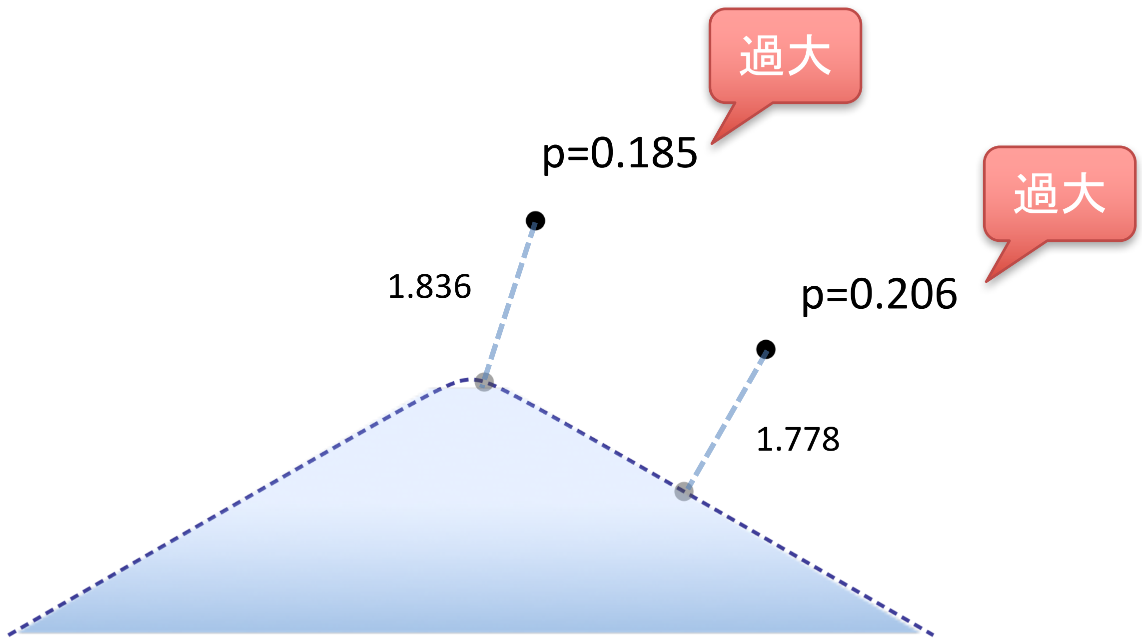
$$H = \left\{ (u, v) \mid v \le -h(u), u \in \mathbb{R}^q \right\}$$

region: $H = \mathcal{R}(h)$ boundary surface: $\partial H = \mathcal{B}(h)$

Null hypothesis: $\mu \in H$ v.s. Alternative hypothesis: $\mu \notin H$

Chi-square test (very conservative)

distance^2 ~ chi-square distribution with df=2



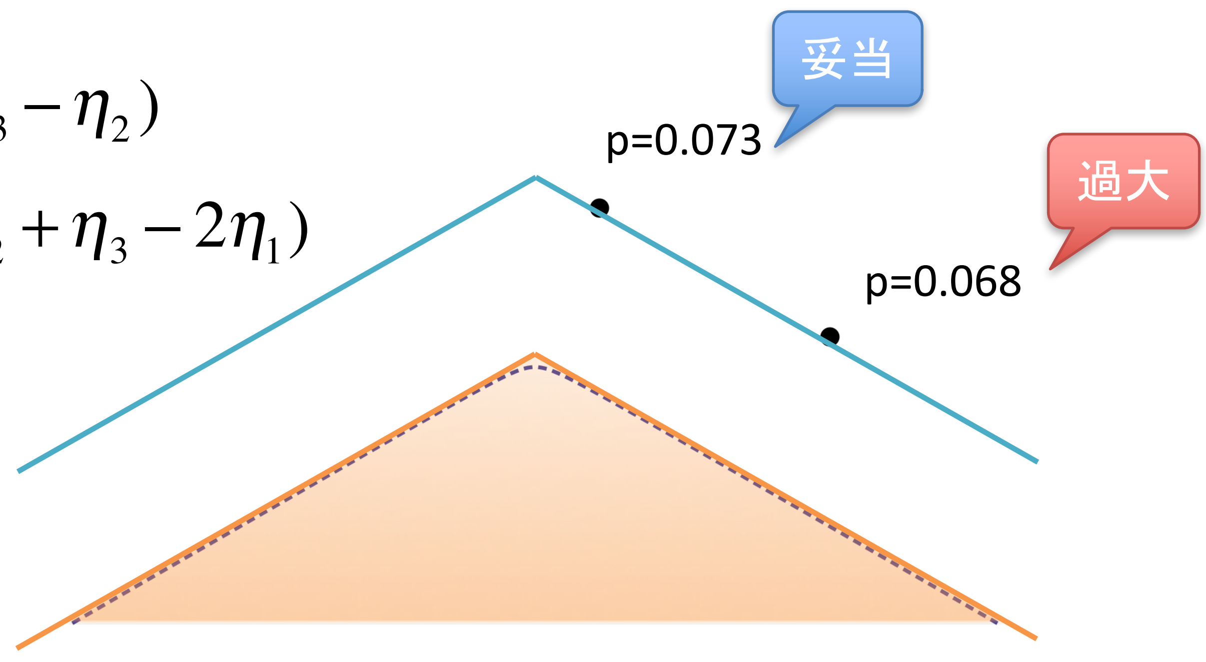
Multiple Comparison (conservative)

$$\bar{X} \sim N_3(\eta, I_3/n) \quad \Leftrightarrow \quad Y \sim N_2(\mu, I_2)$$

$$\eta_1 \geq \eta_2, \eta_1 \geq \eta_3 \quad \Leftrightarrow \quad v \leq -|u|/\sqrt{3}$$

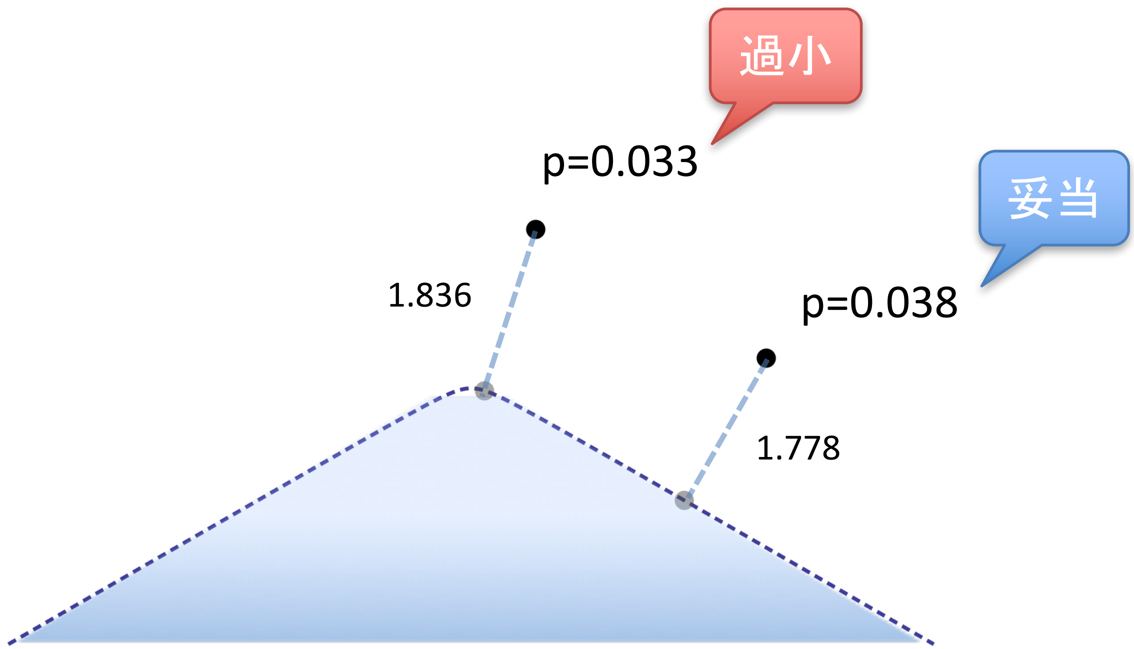
$$u = \sqrt{n/2}(\eta_3 - \eta_2)$$

$$v = \sqrt{n/6}(\eta_2 + \eta_3 - 2\eta_1)$$



Singed LR test (rejecting too much)

distance ~ N(0,1)



Bootstrap probability (=Bayesian PP)

$$Y^* \sim N_{q+1}(y, \sigma^2 I_{q+1}) \qquad \sigma^2 = 1$$

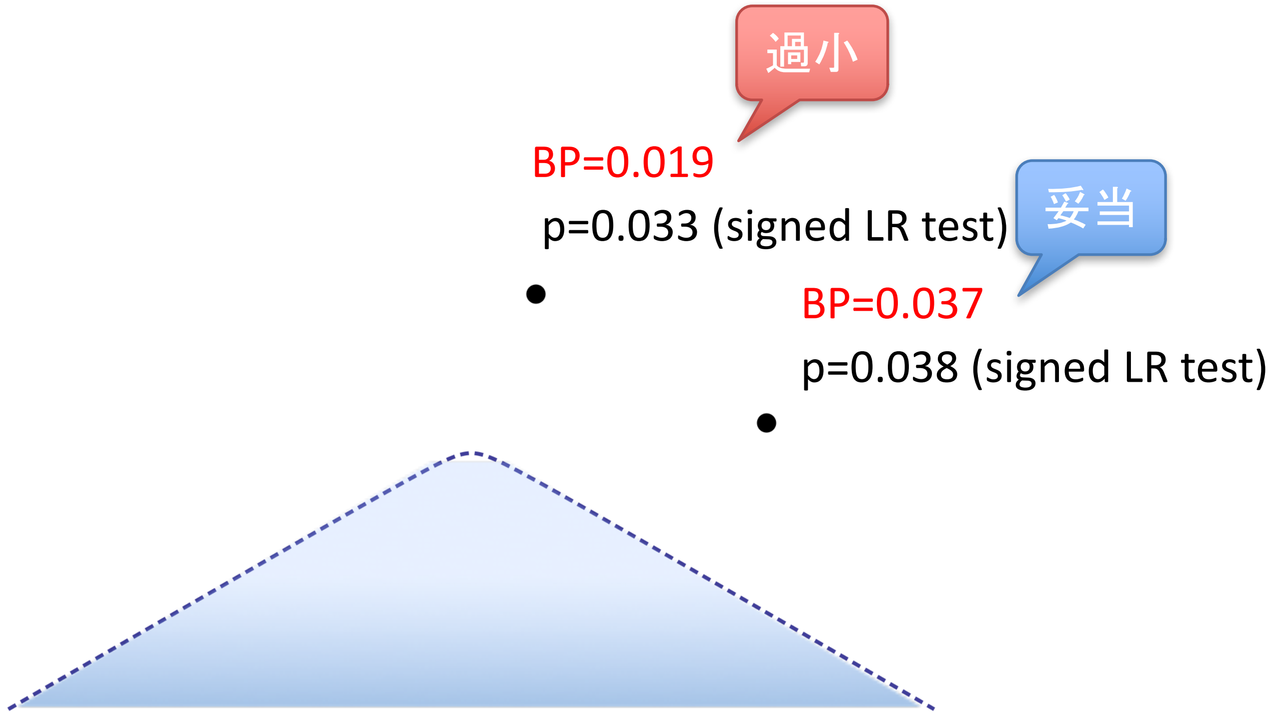
$$Y^{*1}, \ldots, Y^{*B} \quad \Rightarrow \quad \widehat{\mathrm{BP}}_{\sigma^2}(H|y) = \frac{\#\{Y^{*b} \in H, b = 1, \ldots, B\}}{B}$$

$$\mathrm{BP}_{\sigma^2}(H|y) = P(Y^* \in H|y)$$

BP is interpreted as the Bayesian posterior probability of H
if the prior distribution of mu is uniform.

Efron and Tibshirani (1998)

BP is even worse



Double bootstrap probability

Projection of y onto the boundary surface:

$$\hat{\mu}(H|y) = \arg\min_{\mu \in \partial H} \|y - \mu\|$$

Adjusting BP using resampling from the projection

$$Y^+ \sim N_{q+1}(\hat{\mu}(H|y), \tau^2 I_{q+1}) \qquad \tau^2 = 1$$

$$\mathrm{DBP}_{\tau^2,\sigma^2}(H|y) = P_{\tau^2}\left[\mathrm{BP}_{\sigma^2}(H|Y^+) \le \mathrm{BP}_{\sigma^2}(H|y) \mid \hat{\mu}(H|y)\right]$$

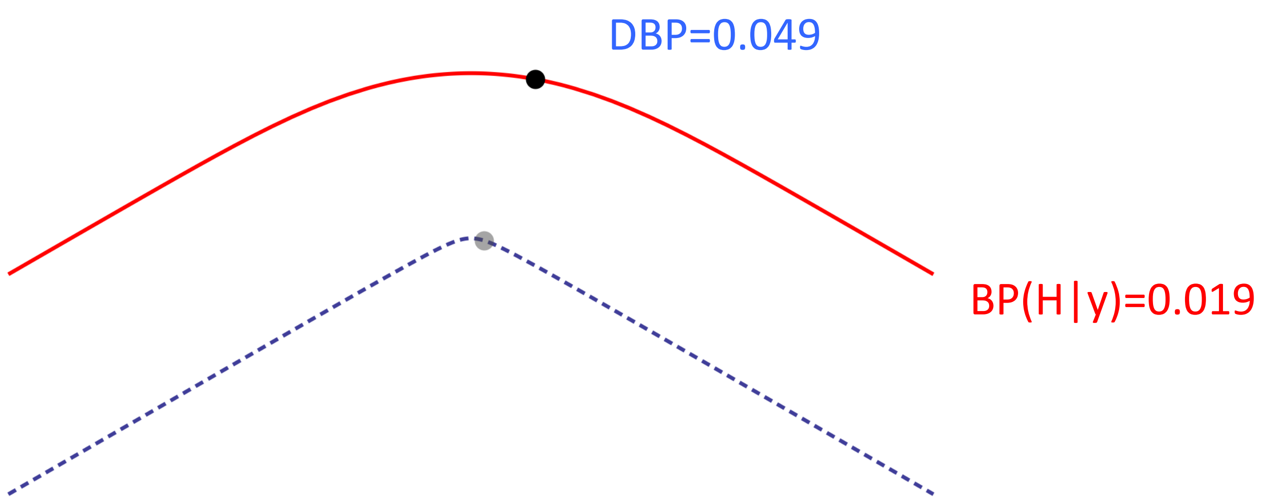
Hall (1992), Efron and Tibshirani (1998)

contour surface of BP=0.019

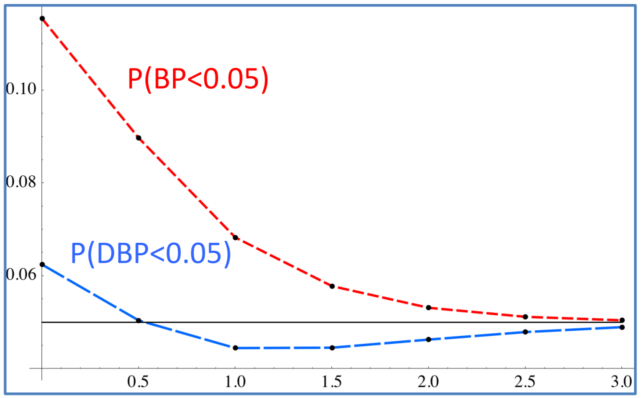
Computing DBP:

$$Y^+ \sim N_2(\hat{\mu}, I_2)$$

$$\mathrm{DBP} = P\Big[\mathrm{BP}(H|Y^+) \leq 0.019 \mid \hat{\mu}\Big]$$

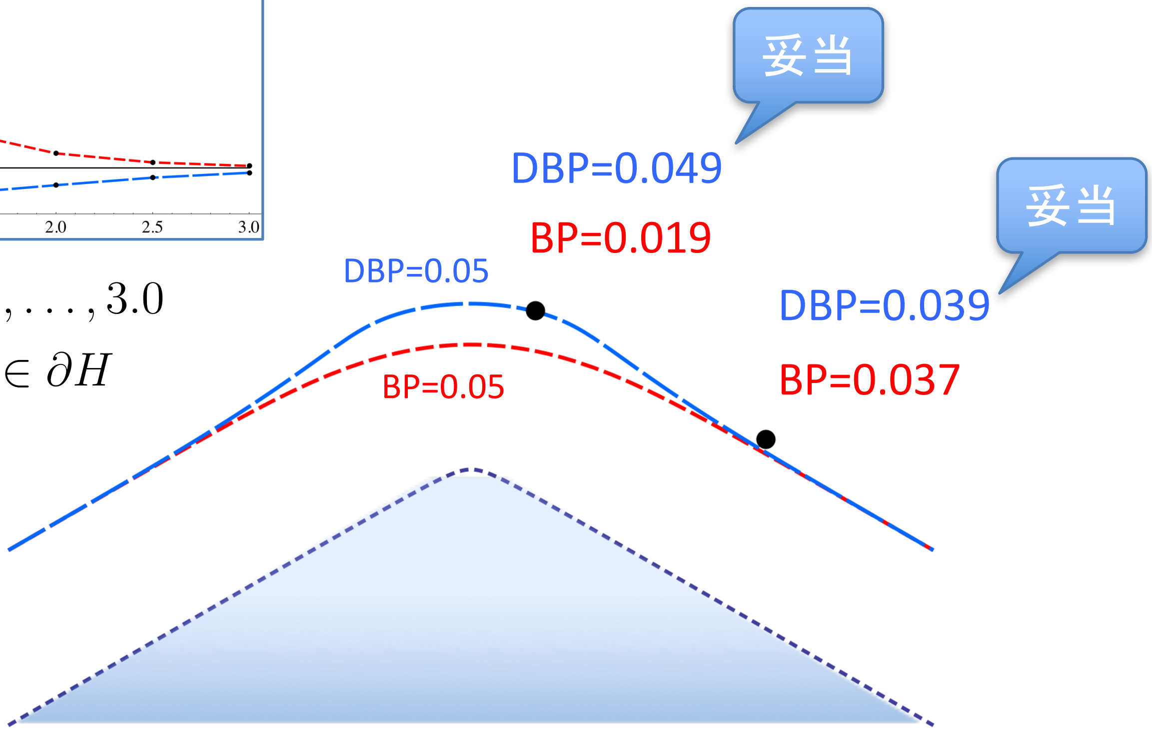


DBP adjusts the bias of BP



$$\theta = 0.0, 0.5, 1.0, \ldots, 3.0$$

$$\mu = (\theta, -h(\theta)) \in \partial H$$



Approximately unbiased p-values via Multiscale bootstrap

m out of n bootstrap : Politis and Romano (1994), Bickel et al. (1997)

$$\mathcal{X} = \{x_1, \ldots, x_n\} \Rightarrow \mathcal{X}^* = \{x_1^*, \ldots, x_m^*\}$$

The idea of multiscale bootstrap : Shimodaira (2002, 2004, 2008)

$$\sigma^2 = \frac{n}{m}$$

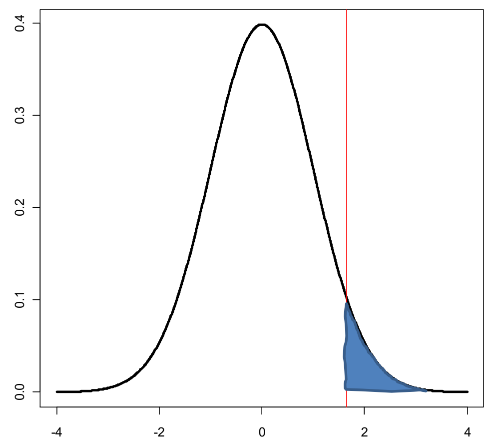
We compute BP for $\sigma_1^2, \ldots, \sigma_S^2$ and extrapolate BP to $\sigma^2 = -1$

(equivalently $m = -n$)

The BP with m = -n is denoted as AU (= Approximately Unbiased)

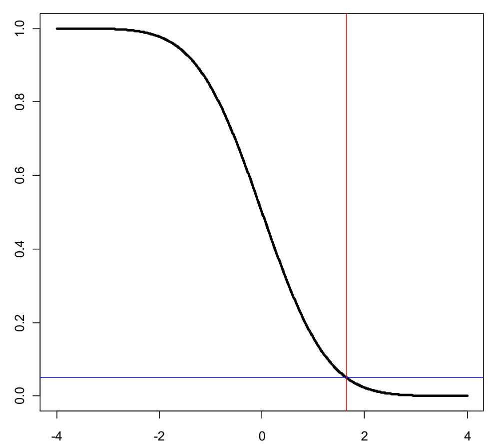
正規分布の上側確率

$$\phi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$



$$\bar{\Phi}(z) = \int_z^\infty \phi(x)dx$$

$\bar{\Phi}(1.64) = 0.05$

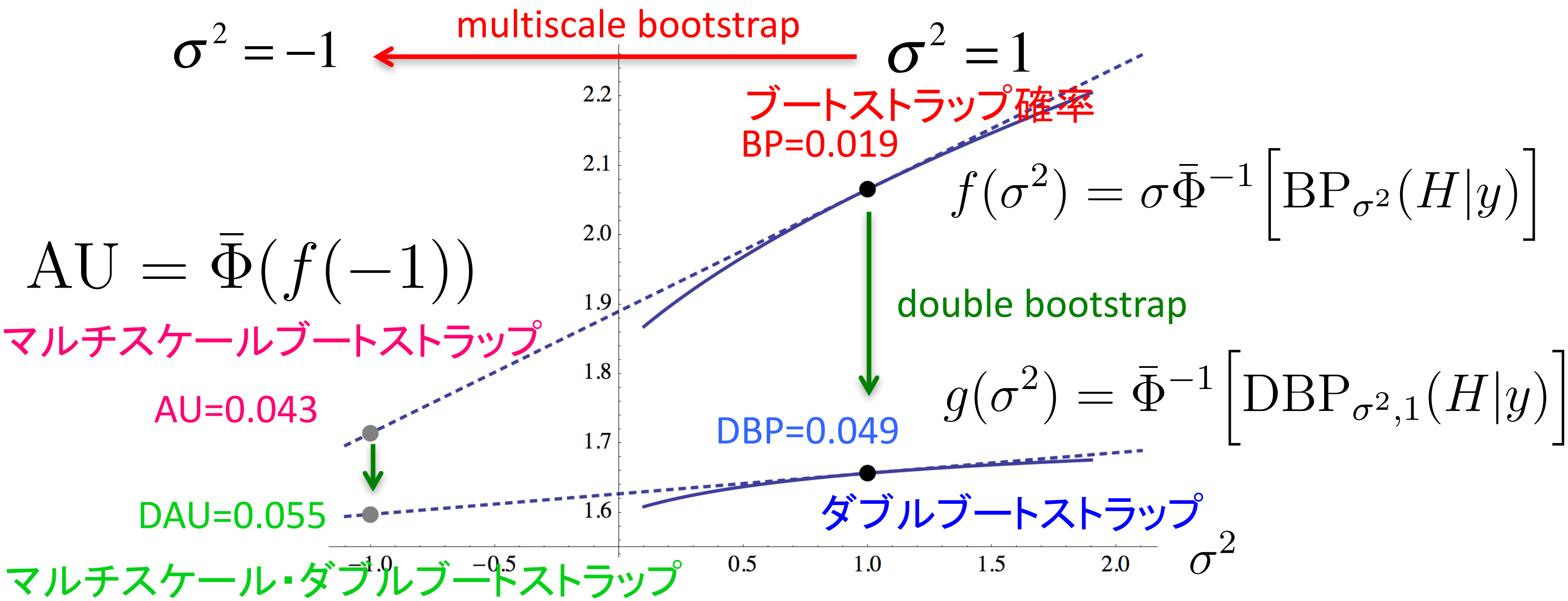


1.64

m=-n　への外挿

Extrapolation to sigma^2=-1

$$\bar{\Phi}(z) = 1 - \Phi(z) = \int_z^\infty \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}\, dx$$

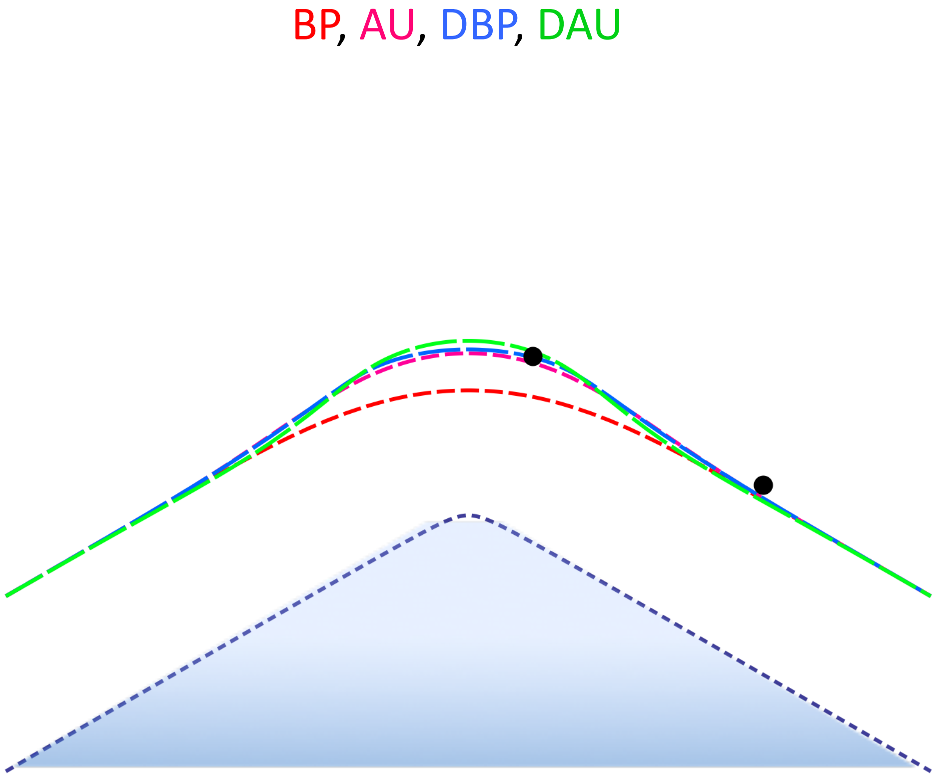


$$\mathrm{DAU} = \bar{\Phi}(g(-1))$$

We apply the multiscale bootstrap to DBP for getting DAU

Equivalently, we could say applying double bootstrap to AU for getting DAU

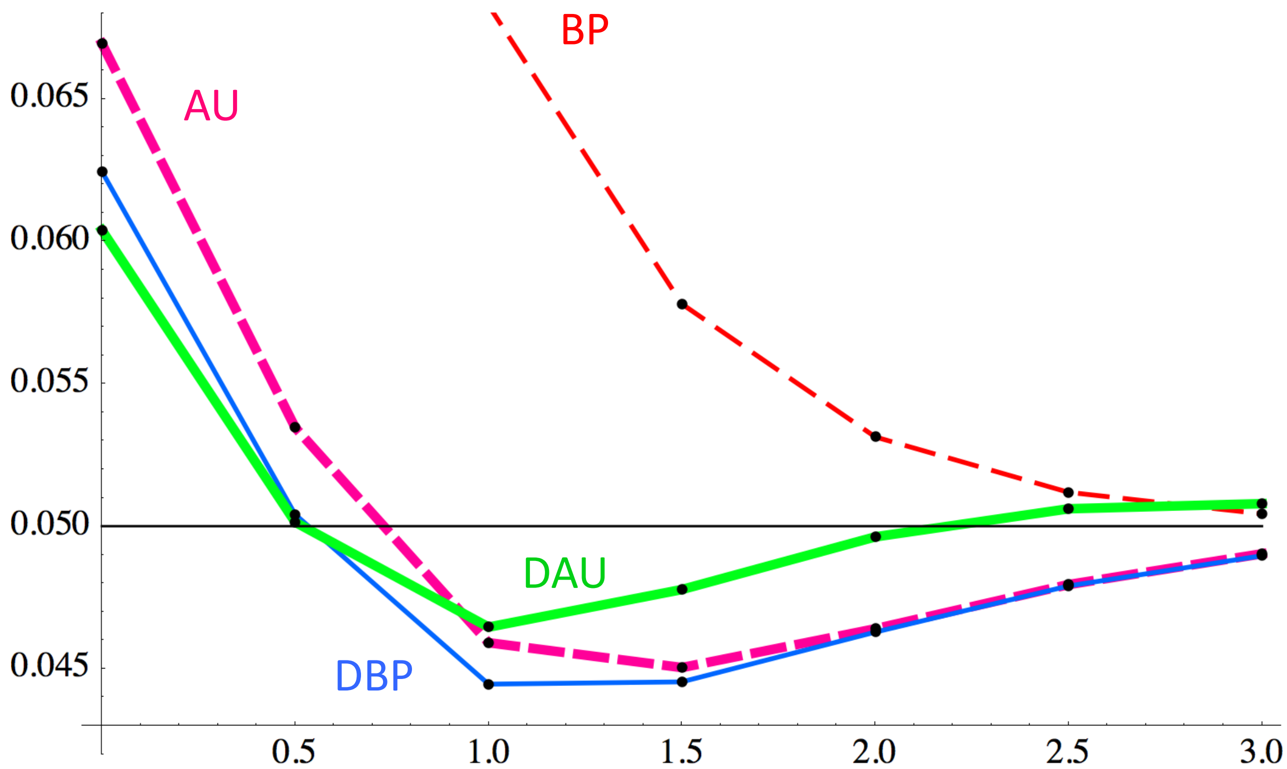
contour curves of p=0.05



DAUの棄却確率は誤差が小さい

Rejection probabilities $P(p<0.05)$

Error: DAU < {DBP, AU} < BP



$\theta = 0.0, 0.5, 1.0, \ldots, 3.0 \qquad \mu = (\theta, -h(\theta)) \in \partial H$

棄却確率 (0.05に近いほど良い)

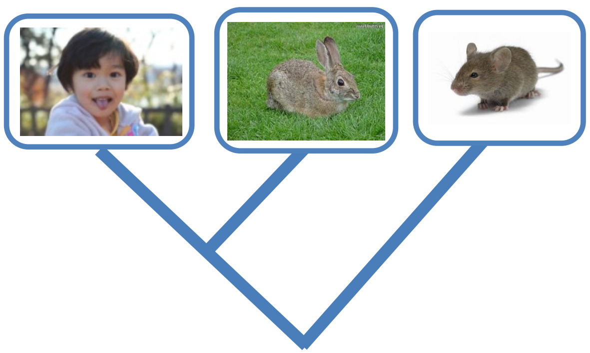
TABLE 2

Rejection pr… es (in percent) at significance level $\alpha = 5\%$.

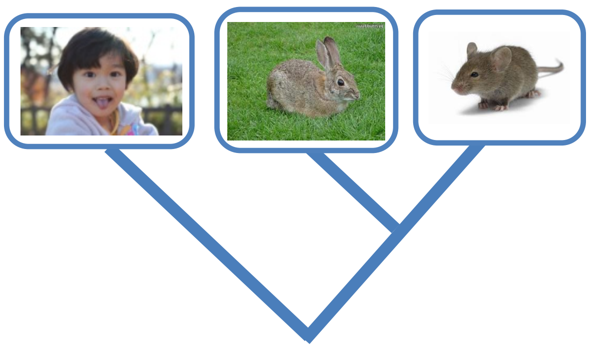
u	0.0	0.5	1.0	1.5	2.0	2.5	3.0
BP	13.39	8.894	6.678	5.676	5.253	5.086	5.027
AU2	7.655	5.171	4.459	4.447	4.628	4.801	4.912
AU3	6.609	4.718	4.493	4.746	4.982	5.080	5.081
DBP	6.619	4.590	4.202	4.364	4.610	4.795	4.905
DAU	6.476	4.660	4.481	4.746	4.981	5.084	5.092
MCB	5.000	3.340	2.880	2.783	2.768	2.766	2.766

過大 妥当 妥当 過小

New Discovery?

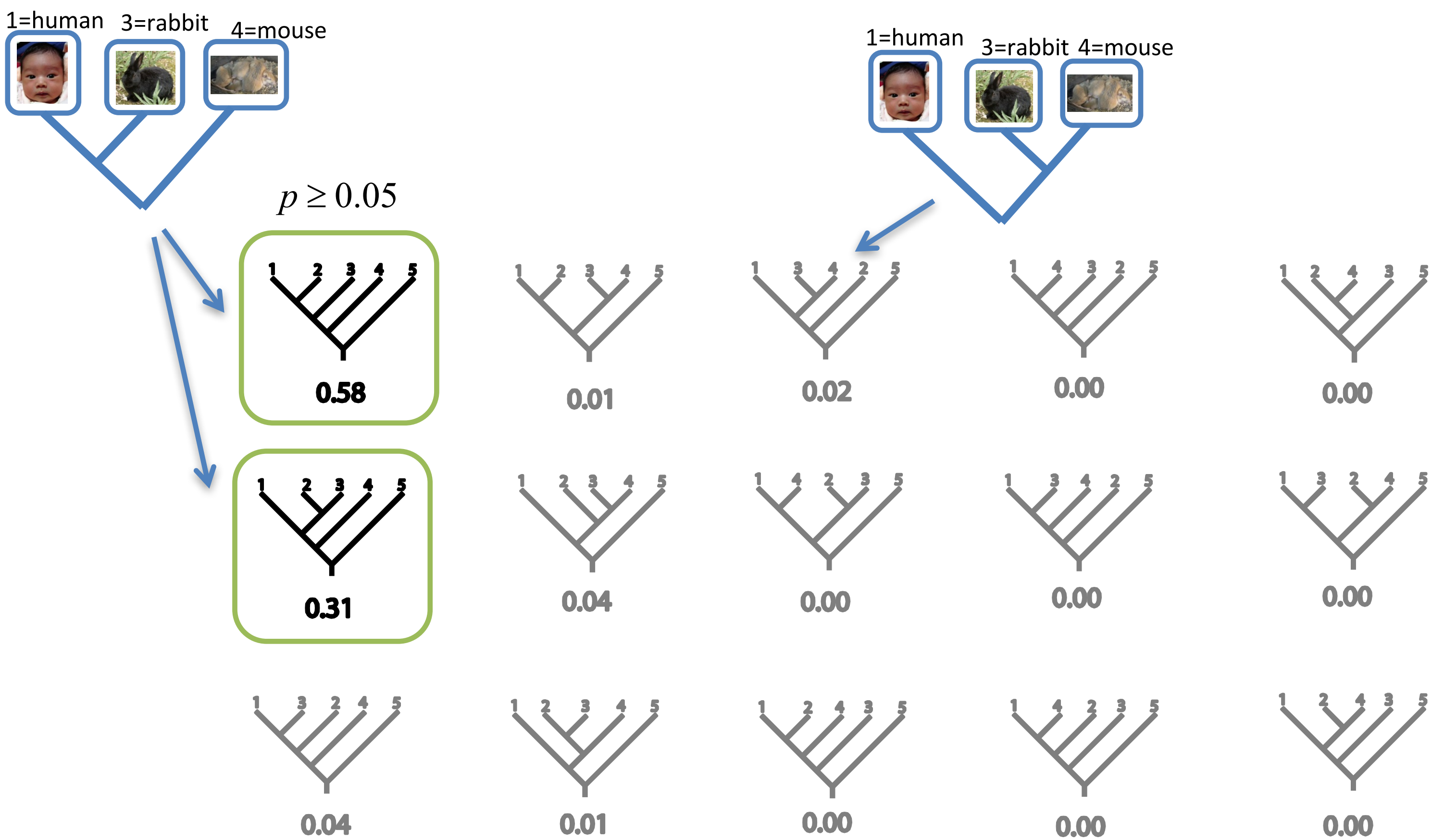


58%



2%

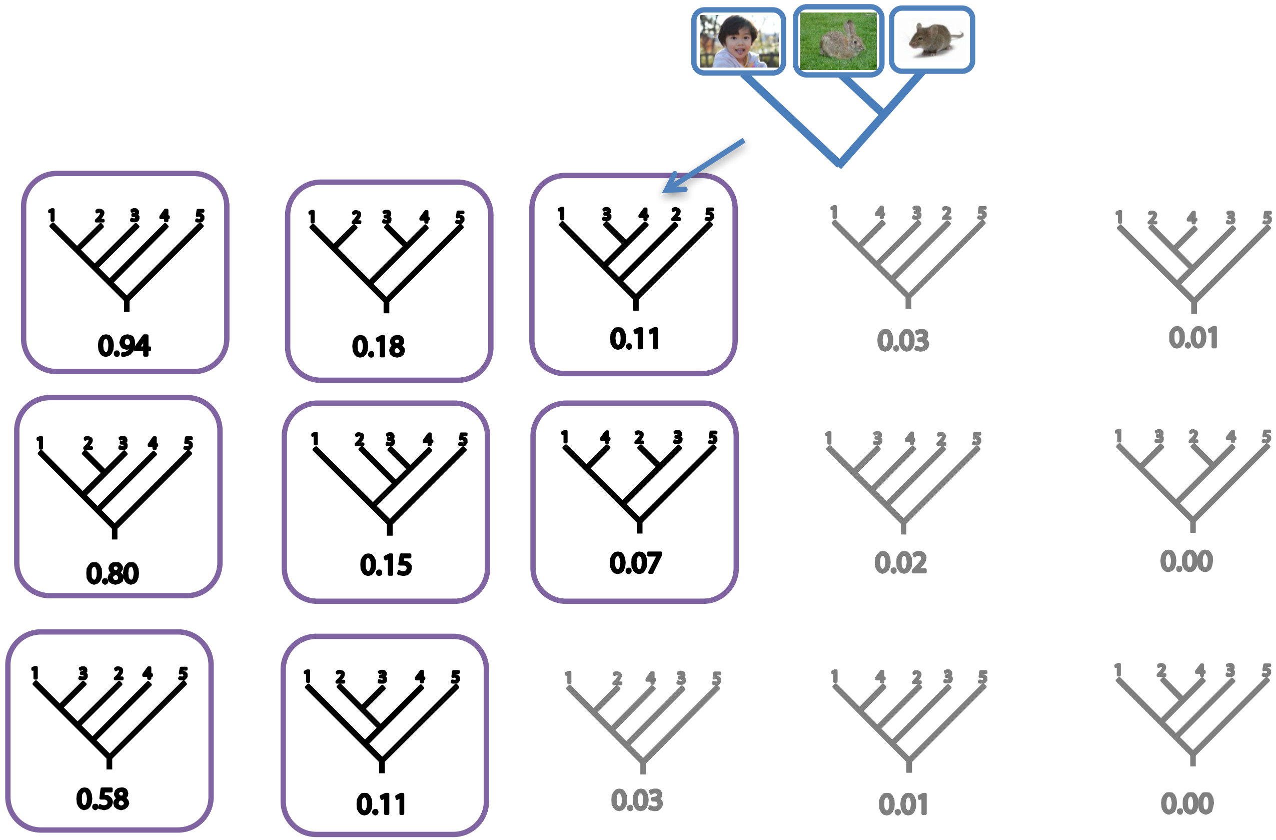
ベイズの事後確率



ブートストラップ法（m=n)で計算

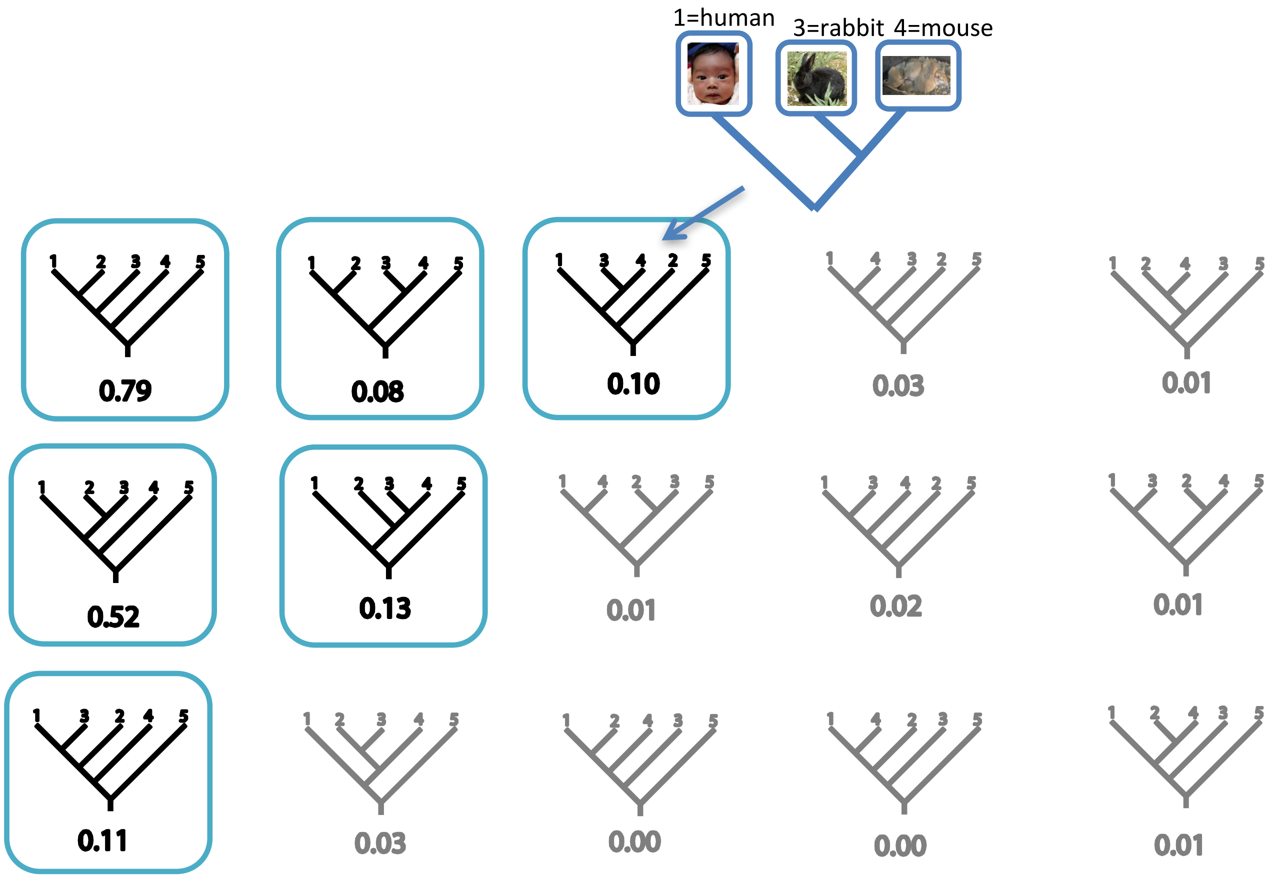
Shimodaira-Hasegawa testは安全すぎる

SH ≥ 0.05



対数尤度に多重比較法を適用してモデル選択の多重性を調整

頻度論のp-値 (近似的に不偏 AU)

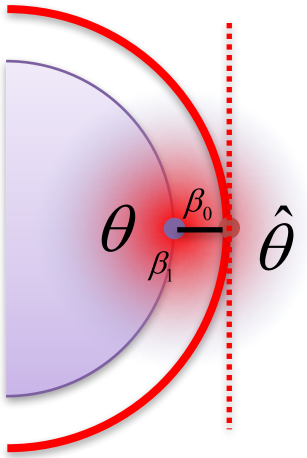


マルチスケール・ブートストラップ法（m=-n)で計算

曲率を反転するとベイズは頻度論

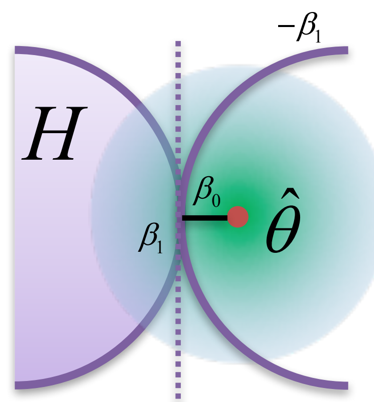
頻度論のp-値

Jerzy Neyman
(1894-1981)
頻度論



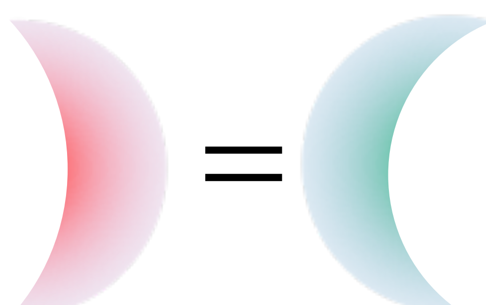
$$AU = \bar{\Phi}\left(\beta_0 - \beta_1\right) + O(n^{-3/2})$$

ベイズの事後確率



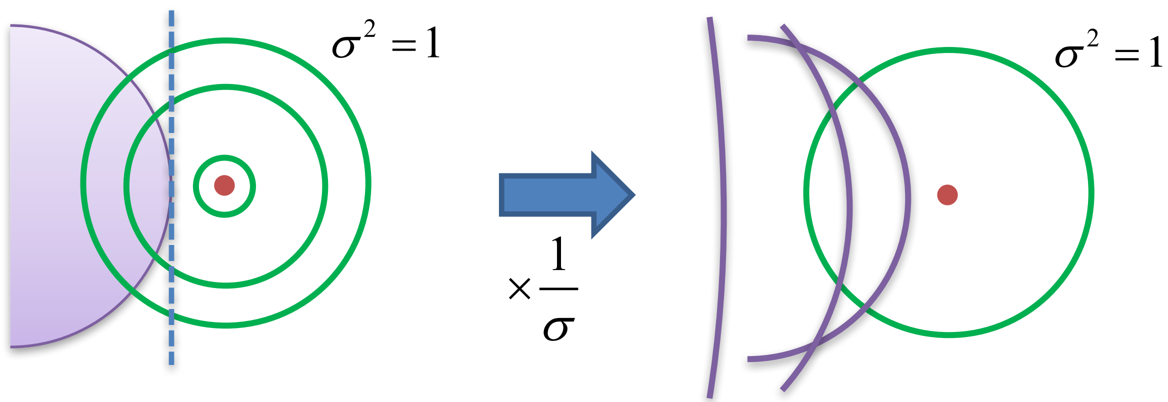
Thomas Bayes
(1702-1761)
ベイズ統計学

$$BP = \bar{\Phi}\left(\beta_0 + \beta_1\right) + O(n^{-3/2})$$



Rescaling the whole picture

Shimodaira (2002)



$$BP = \bar{\Phi}\left(\beta_0 + \beta_1\right) + O(n^{-3/2})$$

$$BP(\sigma^2) = \bar{\Phi}\left[\frac{\beta_0}{\sigma} + \beta_1 \sigma\right] + O(n^{-3/2})$$

$$NBP(\sigma^2) = \bar{\Phi}\left\{\sigma\, \bar{\Phi}^{-1}\left(BP(\sigma^2)\right)\right\} = \bar{\Phi}\left(\beta_0 + \beta_1 \sigma^2\right) + O(n^{-3/2})$$

ベイズと頻度論のギャップを埋める

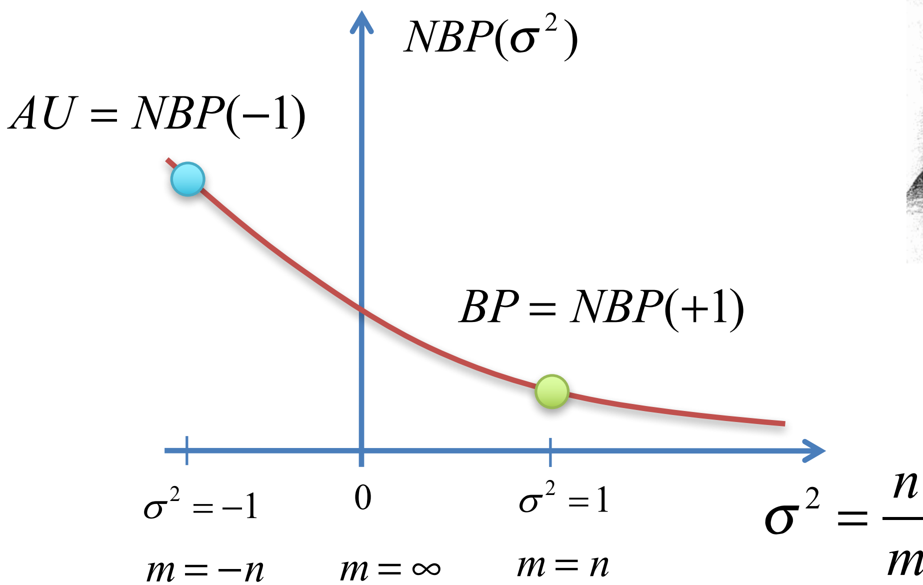
$$NBP(\sigma^2) \triangleq \bar{\Phi}\left\{\sigma\,\bar{\Phi}^{-1}\left(BP(\sigma^2)\right)\right\}$$

正規化したブートストラップ確率(NBP)

スケーリング則

Jerzy Neyman
(1894-1981)

頻度論

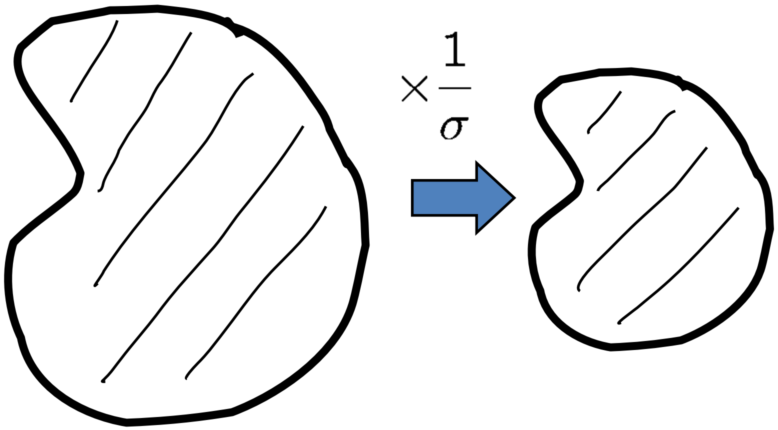


Thomas Bayes
(1702-1761)

ベイズ統計学

AUの計算手順： いくつかのm>0でBPを計算して，NBPに変換してからm=-nへ外挿

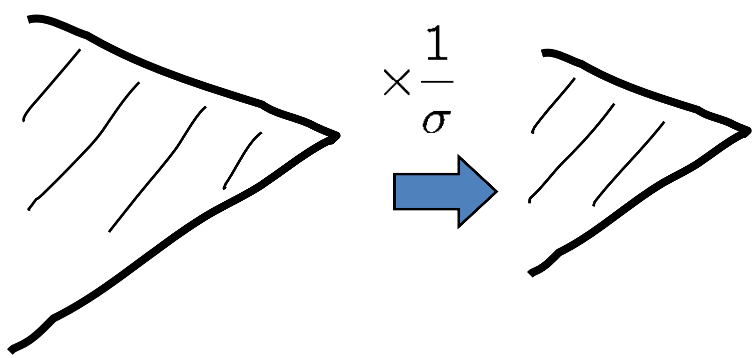
We can’t compute nBP(-1) for cones



smooth surface

$$BP(\sigma^2) \approx \bar{\Phi}\left[\frac{\beta_0}{\sigma} + \beta_1\sigma\right]$$

$$nBP(\sigma^2) \approx \bar{\Phi}\left(\beta_0 + \beta_1\sigma^2\right)$$



cone

$$BP(\sigma^2) \approx \bar{\Phi}\left[\frac{\beta_0}{\sigma} + \beta_1\right]$$

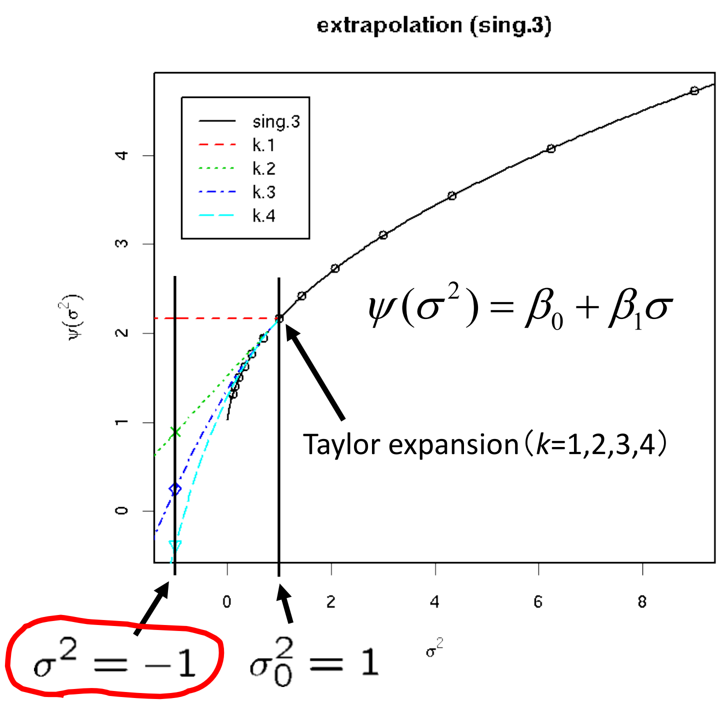
$$nBP(\sigma^2) \approx \bar{\Phi}\left(\beta_0 + \beta_1\sigma\right)$$

Taylor expansion of nBP using k terms

Shimodaira (2008)

$$nBP_k(\sigma^2) = \bar{\Phi}\left[\sum_{j=0}^{k-1} \frac{(\sigma^2 - \sigma_0^2)^j}{j!} \left. \frac{\partial^j \psi(\sigma^2)}{\partial(\sigma^2)^j} \right|_{\sigma_0^2} \right]$$

$$\mathrm{AU}_k = nBP_k(-1)$$



Scaling-law and geometry

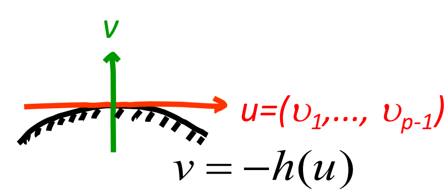
Shimodaira (2008)

$$NBP(\sigma^2) = \bar{\Phi}\left(\beta_0 + \beta_1\sigma^2 + \beta_2\sigma^4 + \beta_3\sigma^6 + \cdots\right) + O(h^2)$$

distance   mean curvature

$$\text{p-value} = \bar{\Phi}\left(\beta_0 - \beta_1 + \beta_2 - \beta_3 + \cdots\right) + O(h^2)$$

$$\beta_j(u) = \frac{1}{2^j j!} \sum_{j_1+\cdots+j_{p-1}=j} \frac{j!}{j_1!\cdots j_{p-1}!} \frac{\partial^{2j} h(u)}{\partial u_1^{2j_1} \cdots \partial u_{p-1}^{2j_{p-1}}}$$



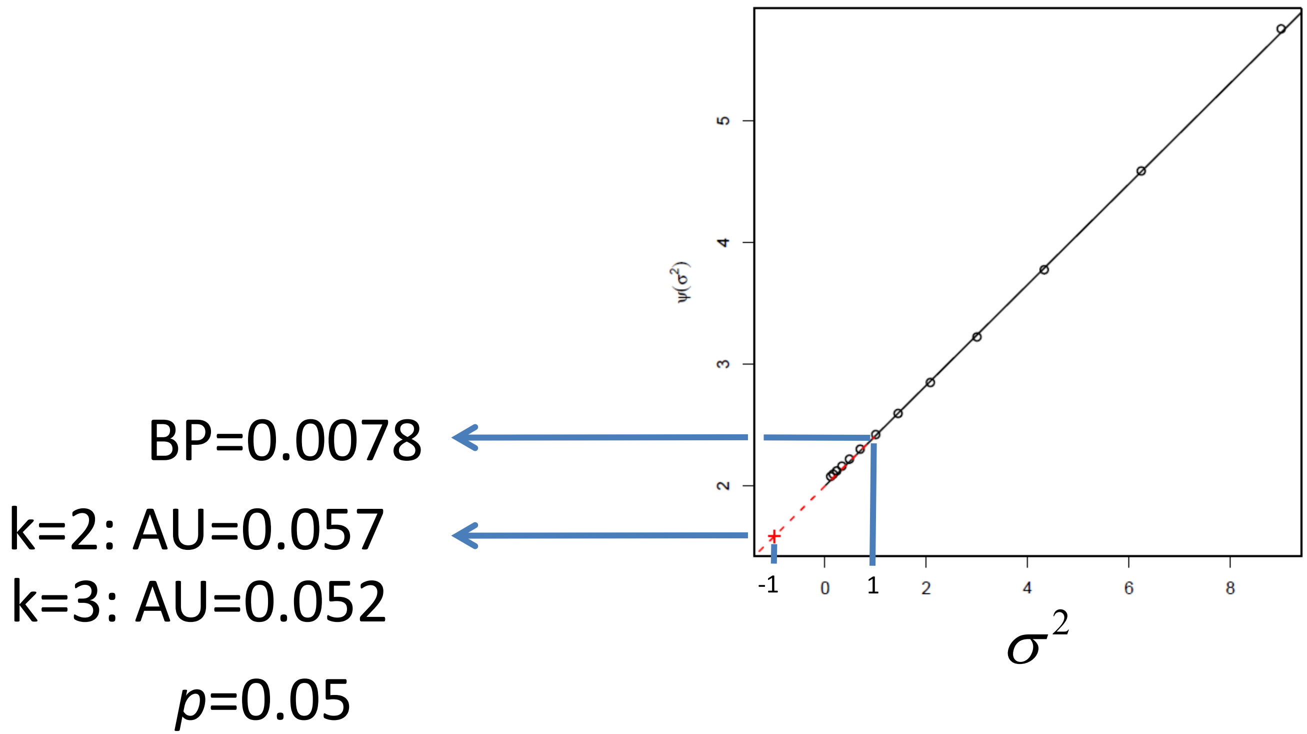
Using a new asymptotic theory with “nearly flat surface h” instead of large n.

Extrapolating NBP to m=-n

$$NBP(\sigma^2) \triangleq \bar{\Phi}\left\{\sigma\, \bar{\Phi}^{-1}\left(BP(\sigma^2)\right)\right\}$$

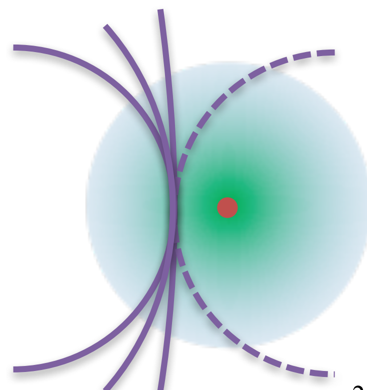
Plotting : $\sigma\, \bar{\Phi}^{-1}\left(BP(\sigma^2)\right)$

Fitting a model : $\psi(\sigma^2) = \beta_0 + \beta_1\sigma^2 + \beta_2\sigma^4 + \cdots + \beta_{k-1}\sigma^{2(k-1)}$



What NBP is calculating ?

Shimodaira (2008)



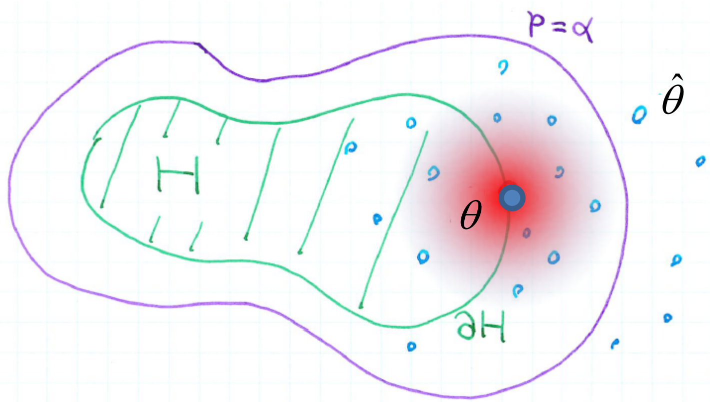
$$NBP(\sigma^2) = \bar{\Phi}\left(\beta_0 + \underbrace{\beta_1\sigma^2}_{\text{curvature}}\right) + O(n^{-3/2})$$

$$NBP(-1) = p\text{-value} + O(n^{-3/2})$$

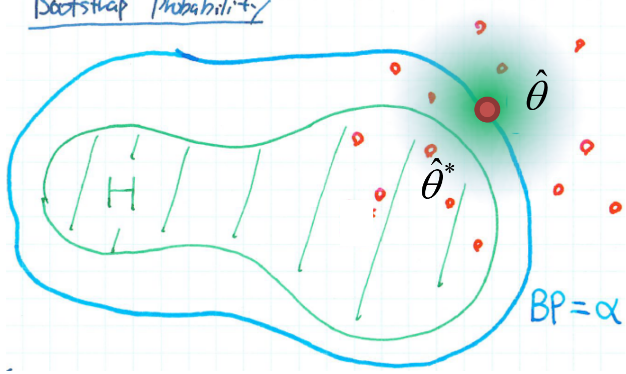
What is an unbiased test?

The p-value of an Unbiased Test (“similar” on the boundary)

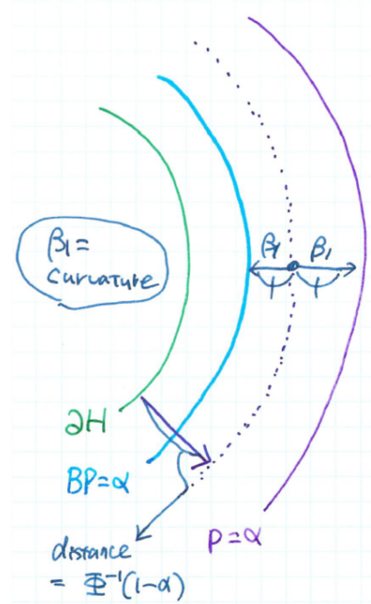
$$P\left\{p(\hat{\theta}) < \alpha \mid \theta\right\} = \alpha, \quad {}^{\forall}\theta \in \partial H, \quad 0 < \alpha < 1$$



Bootstrap Probability

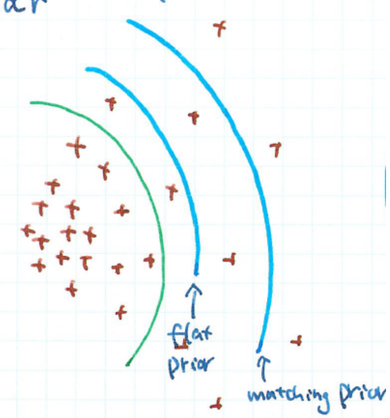


Geometry



Probability Matching Prior

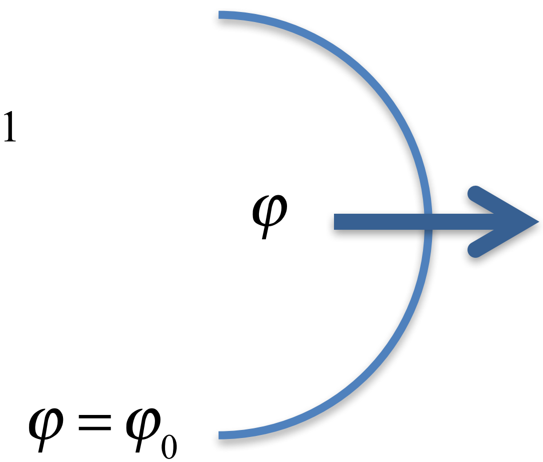
$$\frac{d \log \pi}{dr} = -2\beta_1$$



Matching priors

$$\theta \leftrightarrow (\varphi, \lambda) \qquad \varphi \in \mathbb{R}, \lambda \in \mathbb{R}^{p-1}$$

$$H = \left\{ \theta : \varphi \le \varphi_0 \right\}$$



Tibshirani (1989) assumes orthogonality $I_{\varphi\lambda}(\varphi, \lambda) = 0$

$$\pi(\theta) = g(\lambda) I_{\varphi\varphi}^{1/2}(\varphi, \lambda) \,|\, J(\varphi, \lambda) \,|^{-1}$$

$$\frac{d \log \pi(\theta)}{d\varphi} = -2\beta_1$$

(curvature of the boundary surface of H)

$$\beta_1 \propto 1 / radius$$

Reweighting the bootstrap by this matching prior makes BP=p-value

Correcting a deviation from normality

Efron (1987), Efron and Tibshirani (1998), Shimodaira (2004)

$$a = \frac{1}{6} \frac{E((\hat{\theta} - \theta)^3)}{E((\hat{\theta} - \theta)^2)^{3/2}}$$

acceleration constant

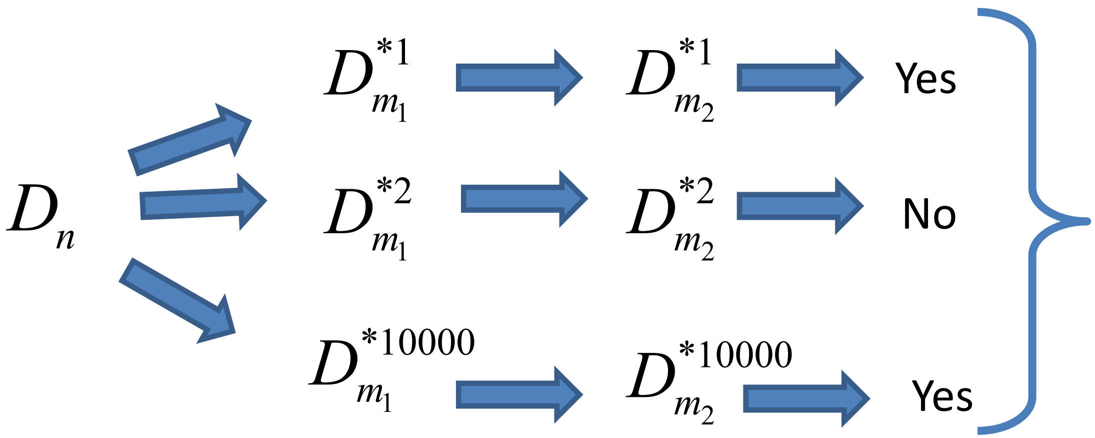
$$nBP(\sigma^2) = \bar{\Phi}\left[(\beta_0 - \beta_1 \sigma^2) \underline{- a(2\beta_0^2 + \sigma^2)} \right] + O(n^{-1})$$

$$p\text{-value} = \bar{\Phi}\left[\beta_0 - \beta_1 \underline{+ a(1 - \beta_0^2)} \right] + O(n^{-1})$$

$$\bar{\Phi}^{-1}(p\text{-value}) - \bar{\Phi}^{-1}(\mathrm{AU}(-1)) = a\beta_0^2 + O(n^{-1})$$

Two-step multiscale bootstrap

Shimodaira (2004)



$$\mathrm{BP}(\sigma_1^2,\sigma_2^2)=\frac{\#\{Yes\}}{10000}$$

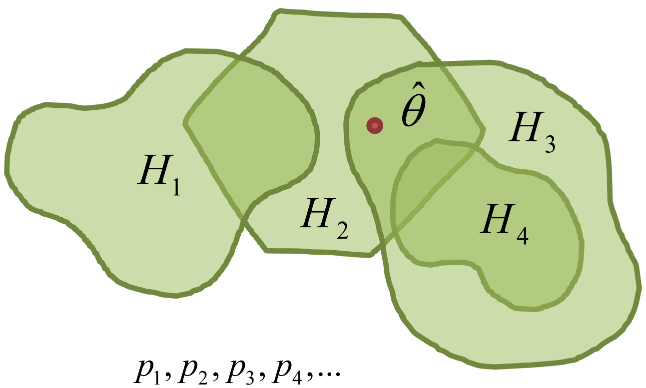
$$=\mathrm{BP}(\sigma^2)+O_p(n^{-1/2})$$

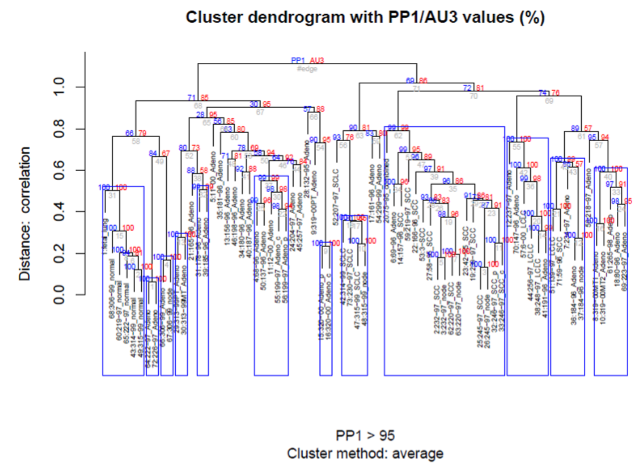
with $\sigma^2=\sigma_1^2+\sigma_2^2$

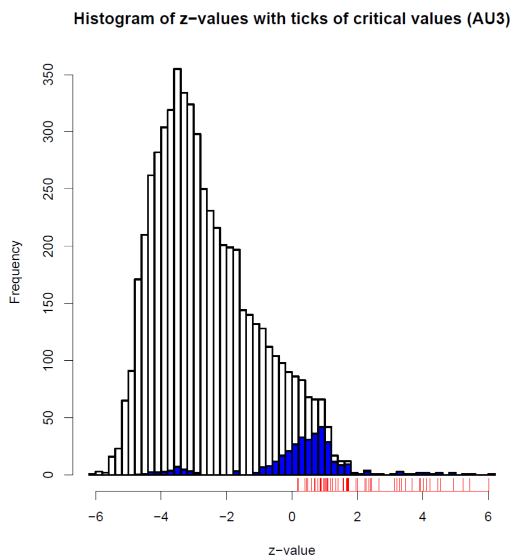
$$\sigma\bar{\Phi}^{-1}(\mathrm{BP}(\sigma_1^2,\sigma_2^2))=\sigma\bar{\Phi}^{-1}(\mathrm{BP}(\sigma^2))+n^{-1/2}a\sigma_1^2\sigma_2^2\sigma^{-4}(\beta_0-\sigma^2)+O_p(n^{-1})$$

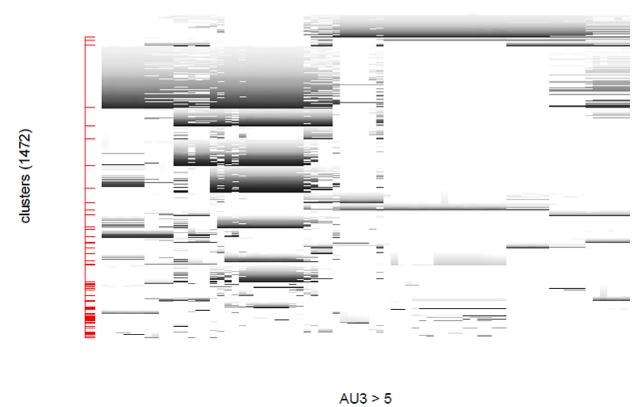
c.f. Three-step multiscale bootstrap estimates six geometrical parameters and gives third-order accuracy

Many hypotheses: FDR, visualization









Asymptotic theory of 4^{th} order accuracy

$$h(u) = \sum_{i=1}^{q}\sum_{j=1}^{q} h_{ij}u_i u_j + \sum_{i=1}^{q}\sum_{j=1}^{q}\sum_{k=1}^{q} h_{ijk}u_i u_j u_k + \cdots$$

$$h_{ij} = \frac{1}{2}\frac{\partial^2 h(u)}{\partial u_i \partial u_j}\Big|_0 = O(n^{-1/2}) \qquad h_{ijk} = \frac{1}{6}\frac{\partial^3 h(u)}{\partial u_i \partial u_j \partial u_k}\Big|_0 = O(n^{-1})$$

曲面の微分係数のスケーリング則

The k-th order derivatives are $O(n^{-(k-1)/2})$ for $k \geq 1$, because the coordinates $u_1, \ldots, u_q$ as well as $h(u)$ are scaled by the factor $\sqrt{n}$

(Class $\mathcal{S}$)

We take care of terms up to $O(n^{-3/2})$ ignoring $O(n^{-2})$

$$h(u) \simeq h_0 + h_i u_i + h_{ij}u_i u_j + h_{ijk}u_i u_j u_k + h_{ijkl}u_i u_j u_k u_l$$

$$h_0 = O(1),\ h_i = O(n^{-1}),\ h_{ij} = O(n^{-1/2}),\ h_{ijk} = O(n^{-1}),\ h_{ijkl} = O(n^{-3/2})$$

Thm: Asymptotic expansion of BP1

$$\mathrm{BP}_1(H|y) \simeq 1 - \Phi(\beta_0 + \beta_1 + \beta_2)$$

Proved by a simple argument of Taylor expansion and integration.

data point $\quad y = (0, \lambda_0 - h_0)$

signed distance $\quad \beta_0 = \lambda_0 = O(1)$

curvature + ... $\quad \beta_1 = \gamma_1 - \lambda_0\gamma_2 + \frac{4}{3}\lambda_0^2\gamma_3 = O(n^{-1/2})$

fourth-order terms
$$\begin{cases} \beta_2 = 3\gamma_4 - \gamma_1\gamma_2 - \frac{4}{3}\gamma_3 = O(n^{-3/2}) \\ \beta_3 = 6\gamma_4 - 2\gamma_1\gamma_2 - 4\gamma_3 = O(n^{-3/2}) \end{cases}$$

$$\gamma_1 = \frac{1}{2}\frac{\partial^2 h(u)}{\partial u_i \partial u_i}\Big|_0$$

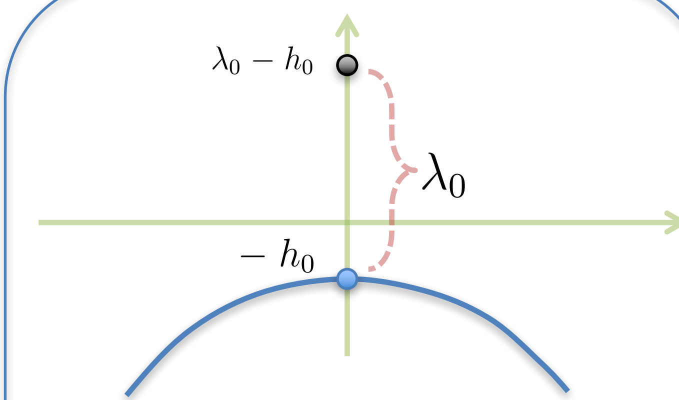
mean curvature of the surface

仮説曲面の平均曲率

$$\beta_3 = \frac{1}{2}\frac{\partial^2 \gamma_1(h,u)}{\partial u_i \partial u_i}\Big|_0$$

mean curvature of the mean curvature

平均曲率の平均曲率



$$\gamma_1 = h_{ii} = O(n^{-1/2})$$

$$\gamma_2 = h_{ij}h_{ij} = O(n^{-1})$$

$$\gamma_3 = h_{ij}h_{jk}h_{ki} = O(n^{-3/2})$$

$$\gamma_4 = h_{iijj} = O(n^{-3/2})$$

ブートストラップ確率のスケーリング則

Thm: scaling law of BP

$$\mathrm{BP}_{\sigma^2}(H|y) \simeq 1 - \Phi\left[\beta_0\sigma^{-1} + \beta_1\sigma + \beta_2\sigma^3\right]$$

$$\mathrm{NBP}_{\sigma^2}(H|y) = \Phi\left[\sigma\Phi^{-1}(\mathrm{BP}_{\sigma^2}(H|y))\right]$$

$$\mathrm{NBP}_{\sigma^2}(H|y) \simeq \bar{\Phi}\left[\beta_0 + \beta_1\sigma^2 + \beta_2\sigma^4\right]$$

Proved by a simple rescaling argument.

$$\mathrm{BP}_{\sigma^2}(H|y) = \mathrm{BP}_1(H/\sigma|y/\sigma)$$

$$\beta_0 \to \beta_0\sigma^{-1}, \quad \beta_1 \to \beta_1\sigma, \quad \beta_2 \to \beta_2\sigma^3$$

$$\lambda_0 \to \lambda_0/\sigma$$

$$h_0 \to h_0/\sigma, h_i \to h_i, h_{ij} \to \sigma h_{ij}, h_{ijk} \to \sigma^2 h_{ijk}, h_{ijkl} \to \sigma^3 h_{ijkl}$$

$$\gamma_1 \to \sigma\gamma_1, \gamma_2 \to \sigma^2\gamma_2, \gamma_3 \to \sigma^3\gamma_3, \gamma_4 \to \sigma^3\gamma_4$$

バイアスの無い（不偏な）p-値

Thm: unbiased p-value

Def: k-th order accurate p-values should satisfy

$$P\Big[\mathrm{PV}(H|Y) < \alpha \mid \mu\Big] = \alpha + \underbrace{O(n^{-k/2})}_{\text{error}}, \quad \mu \in \partial H$$

Thm: fourth-order accuracy (k=4) is achieved by

$$\mathrm{PV}(H|y) \simeq 1 - \Phi\Big[\beta_0 - \beta_1 - \beta_2 + \beta_3\Big]$$

$O(1)$ $O(n^{-1/2})$ $O(n^{-3/2})$

Corollary: BP is first-order accurate (k=1), AU is third-order accurate (k=3)

$$\mathrm{NBP}_{\sigma^2}(H|y) \simeq \bar{\Phi}\Big[\beta_0 + \beta_1\sigma^2 + \beta_2\sigma^4\Big]$$

$$\mathrm{BP} = \mathrm{PV} + O(n^{-1/2}) \qquad \mathrm{AU} = \mathrm{PV} + O(n^{-3/2})$$

棄却確率

Rejection probabilities of BP and AU

BP is first-order accurate (k=1)

$$P\Big(\mathrm{BP}(H|Y) < \alpha\Big) = \Phi(z_\alpha + \underline{2\gamma_1}) + O(n^{-1}) = \alpha + O(n^{-1/2})$$

$$\boxed{z_\alpha = \Phi^{-1}(\alpha)}$$

mean curvature of the surface

仮説曲面の平均曲率

AU is third-order accurate (k=3)

$$P\Big(\mathrm{AU}(H|Y) < \alpha\Big) \simeq \Phi(z_\alpha + \underline{\tfrac{4}{3}\gamma_3}) = \alpha + O(n^{-3/2})$$

Using q x q hessian matrix $D = \left(\left.\frac{\partial^2 h(u)}{\partial u_i \partial u_j}\right|_0 : i, j = 1, \ldots, q \right)$

$$\gamma_1 = h_{ii} = \tfrac{1}{2}\,\mathrm{tr}(D) \qquad \gamma_3 = h_{ij}h_{jk}h_{ki} = \tfrac{1}{8}\,\mathrm{tr}(D^3)$$

曲面の移動

4.3. Shifting surfaces

We consider shifting $\mathcal{B}(h)$ toward the normal direction. Let $f(u)$ be the normal vector at $(u, -h(u)) \in \mathcal{B}(h)$. For a specified $\lambda \in \mathcal{S}$, we move the point $(u, -h(u))$ by $\lambda(u)$ toward the normal direction. This is expressed as

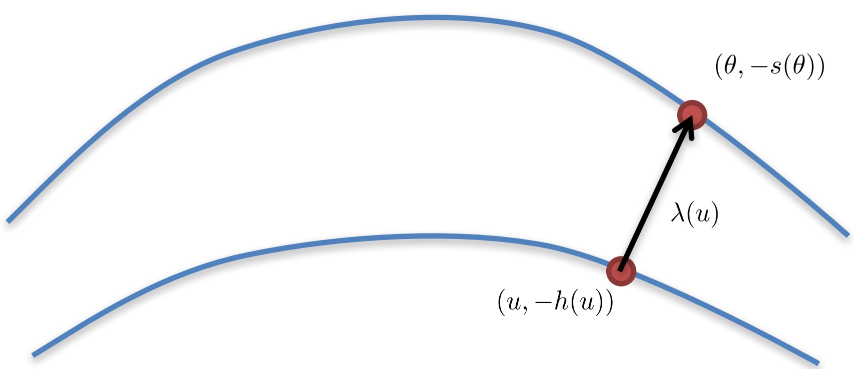
$$(\theta, -s(\theta)) = (u, -h(u)) + \lambda(u)\|f(u)\|^{-1} f(u), \tag{25}$$

where $s(u)$ is some function of $u \in \mathbb{R}^q$, and $\theta \in \mathbb{R}^q$ is used when distinction is needed. We can interpret (25) as

$$\hat{\mu}(H|(\theta, -s(\theta))) = (u, -h(u))$$

with signed distance $\lambda(u)$. For sufficiently large n, such $s(\theta)$ is uniquely defined for each θ, because all the surfaces approach flat as $n \to \infty$. We denote (25) as

$$s = \mathcal{M}(h, \lambda).$$



Lemma 3. *Let* $s = \mathcal{M}(h, \lambda)$ *for* $h \in \mathcal{S}$, $\lambda \in \mathcal{S}$. *If* $\lambda(u)$ *is expressed as*

$$\lambda(u) \simeq \lambda_0 + \lambda_i u_i + \lambda_{ij} u_i u_j$$

with $\lambda_0 = O(1)$, $\lambda_i = O(n^{-1})$, $\lambda_{ij} = O(n^{-3/2})$, *then we have* $s \in \mathcal{S}$ *with coefficients* $s_0 = h_0 - \lambda_0 = O(1)$, $s_i = h_i - \lambda_i - 2\lambda_0 h_{mi}(h_m - \lambda_m) = O(n^{-1})$, $s_{ij} = h_{ij} - \lambda_{ij} - 2\lambda_0 h_{mi} h_{mj} + 4\lambda_0^2 h_{ml} h_{mi} h_{lj} = O(n^{-1/2})$, $s_{ijk} = h_{ijk} - 2\lambda_0(h_{mi}h_{mjk} + h_{mj}h_{mik} + h_{mk}h_{mij}) = O(n^{-1})$, $s_{ijkl} = h_{ijkl} = O(n^{-3/2})$. *The four geometric quantities at* $(0, -s(0))$ *are* $\gamma_1(s, 0) = s_{ii} \simeq \gamma_1 - \lambda_{ii} - 2\lambda_0\gamma_2 + 4\lambda_0^2\gamma_3$, $\gamma_2(s, 0) = s_{ij}s_{ij} \simeq \gamma_2 - 4\lambda_0\gamma_3$, $\gamma_3(s, 0) = s_{ij}s_{jk}s_{ki} \simeq \gamma_3$, $\gamma_4(s, 0) = s_{iijj} \simeq \gamma_4$, *where* $\gamma_i = \gamma_i(h, 0)$, $i = 1, \ldots, 4$.

BPが一定の曲面

5.1. Contour surfaces of bootstrap probability

We consider a surface on which the bootstrap probability remains constant. For $H = \mathcal{R}(h)$ with $h \in \mathcal{S}$, we consider a function $s(u)$ of $u \in \mathbb{R}^q$ satisfying

$$\mathrm{BP}_{\sigma^2}(H|(u, -s(u))) = 1 - \alpha, \quad u \in \mathbb{R}^q,$$

meaning $\mathrm{BP}_{\sigma^2}(H|y) = 1 - \alpha$ is constant for any $y \in \mathcal{B}(s)$. Then, $\mathcal{B}(s)$, as well as s itself, will be called as the *contour surface of the bootstrap probability* of H with variance $\sigma^2 > 0$ at level $1 - \alpha$. In particular, we choose α so that $(0, \lambda_0 - h_0) \in \mathcal{B}(s)$ for a specified $\lambda_0 \in \mathbb{R}$. We denote this contour surface as

$$s = \mathcal{L}_{\sigma^2}(h, \lambda_0).$$

Lemma 4. *Let* $s = \mathcal{L}_{\sigma^2}(h, \lambda_0)$ *for* $h \in \mathcal{S}$, $\lambda_0 \in \mathbb{R}$, *and* $\sigma^2 > 0$. *Then,* s *is expressed as* $s = \mathcal{M}(h, \lambda)$ *by specifying* $\lambda(u) \simeq \lambda_0 + \lambda_i u_i + \lambda_{ij} u_i u_j$ *with* $\lambda_0 = O(1)$,

$$\lambda_i = \sigma^2(-3h_{mmi} + 6\lambda_0 h_{ml} h_{mli}), \quad \lambda_{ij} = \sigma^2(-6h_{mmij} + 2h_{mm} h_{li} h_{lj} + 4h_{ml} h_{mi} h_{lj}). \tag{26}$$

We have $s \in \mathcal{S}$ *with coefficients*

$$\begin{aligned} s_0 &= h_0 - \lambda_0, \quad s_i = h_i - 2\lambda_0 h_m h_{mi} + \sigma^2(3h_{mmi} - 6\lambda_0 h_{ml} h_{mli} - 6\lambda_0 h_{mi} h_{mll}), \\ s_{ij} &= h_{ij} - 2\lambda_0 h_{mi} h_{mj} + 4\lambda_0^2 h_{ml} h_{mi} h_{lj} + \sigma^2(6h_{ijmm} - 2h_{mm} h_{li} h_{lj} - 4h_{ml} h_{mi} h_{lj}), \\ s_{ijk} &= h_{ijk} - 2\lambda_0(h_{mi} h_{mjk} + h_{mj} h_{mik} + h_{mk} h_{mij}), \quad s_{ijkl} = h_{ijkl}. \end{aligned} \tag{27}$$

The four geometric quantities of s *at* $(0, -s(0))$ *are*

$$\begin{aligned} &\gamma_1(s,0) \simeq \gamma_1 - 2\lambda_0\gamma_2 + 4\lambda_0^2\gamma_3 + \sigma^2(6\gamma_4 - 2\gamma_1\gamma_2 - 4\gamma_3), \\ &\gamma_2(s,0) \simeq \gamma_2 - 4\lambda_0\gamma_3, \quad \gamma_3(s,0) \simeq \gamma_3, \quad \gamma_4(s,0) \simeq \gamma_4, \end{aligned} \tag{28}$$

where $\gamma_i = \gamma_i(h, 0)$, $i = 1, \ldots, 4$.

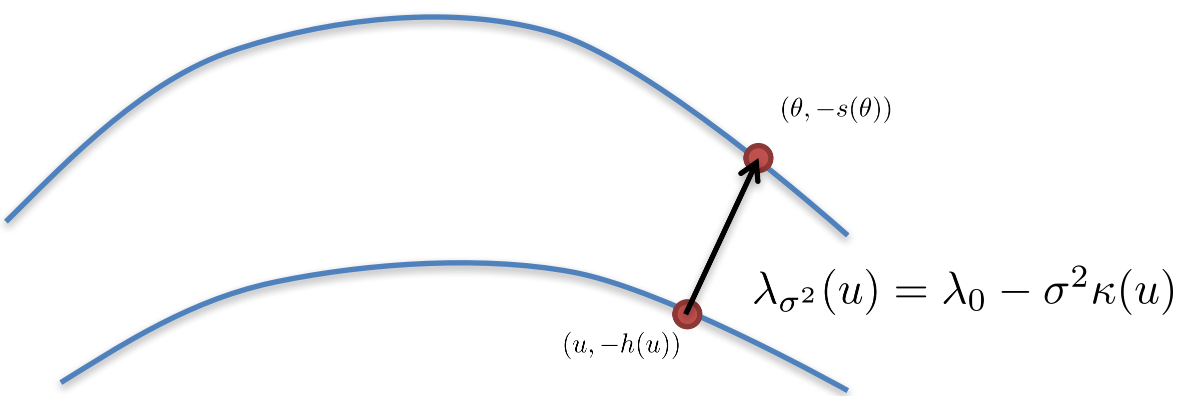
BPの等高線を仮説のシフトと解釈

We denote the $\lambda(u)$ of (26) as $\lambda_{\sigma^2}(u) = \lambda_0 - \sigma^2\kappa(u)$ with

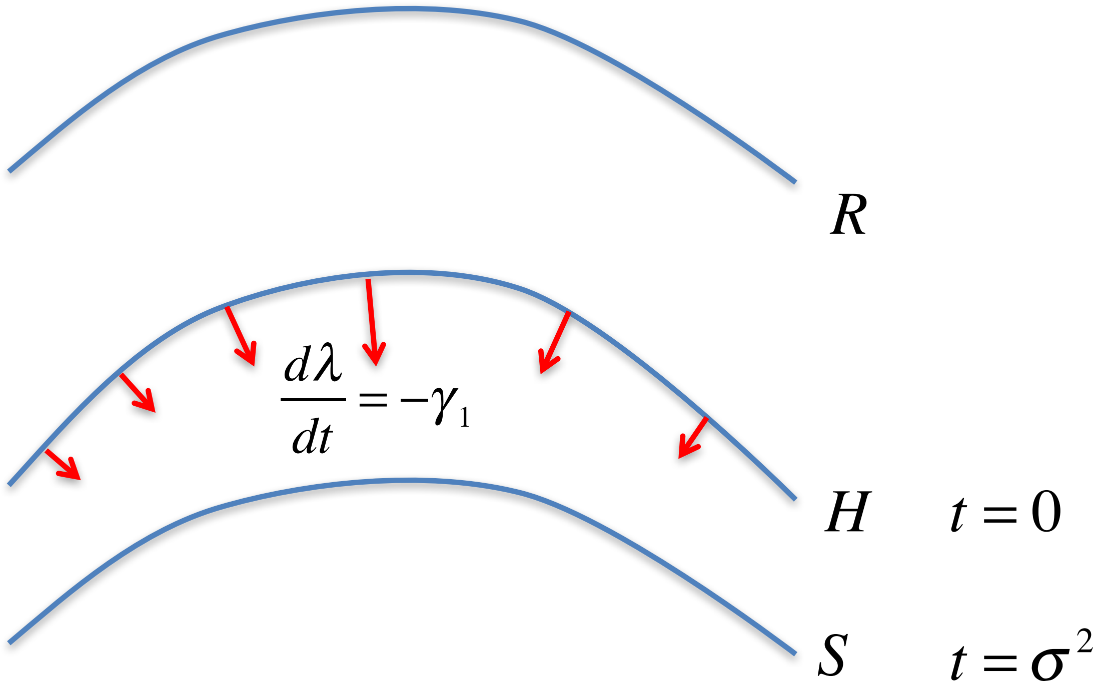
$$\begin{aligned}\kappa(u) &= \gamma_1(h,u) - \gamma_1(h,0) - \lambda_0(\gamma_2(h,u) - \gamma_2(h,0)) \\ &\simeq (3h_{mmi} - 6\lambda_0 h_{ml}h_{mli})u_i + (6h_{mmij} - 2h_{mm}h_{li}h_{lj} - 4h_{ml}h_{mi}h_{lj})u_iu_j. \end{aligned} \tag{29}$$

This also relates to (8) as $(1/2)\partial^2\kappa(u)/\partial u_i\partial u_i|_0 = \beta_3$ or $(1/2)\partial^2\lambda_{\sigma^2}(u)/\partial u_i\partial u_i|_0 = -\sigma^2\beta_3$. The contour surface of $\mathrm{BP}_{\sigma^2}(H|y)$ for $\sigma^2 > 0$ is expressed asymptotically as

$$\mathcal{L}_{\sigma^2}(h,\lambda_0) = \mathcal{M}(h,\lambda_{\sigma^2}),$$

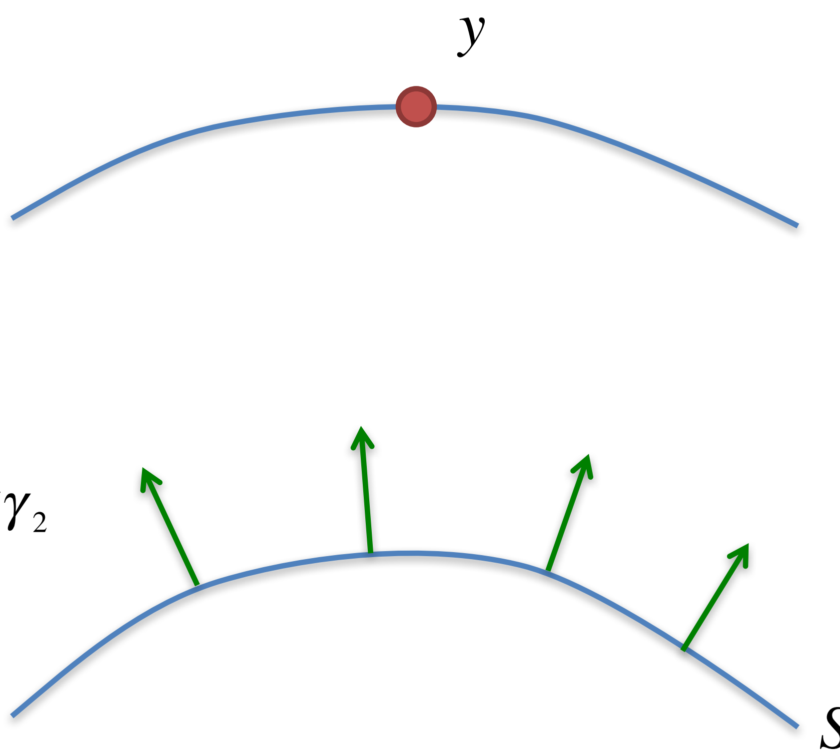


平均曲率流で動かす（3次の議論）



$$NBP_{\sigma^2}(H \mid (u, -s(u)) = 1/2$$

さらに曲面を動かす



$$t = \bar{\Phi}^{-1}(NBP_{\sigma^2}(H \mid y))$$

$$\frac{d\lambda}{dt} = 1 + \sigma^2 \gamma_2$$

$$t = 0$$

$$NBP_{\sigma^2}(H \mid (u, -s(u)) = 1/2$$

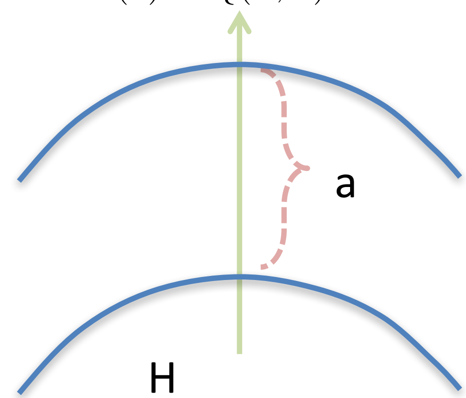
BPの等高線（曲面）のオペレータを定義して証明します

sketch of the proof for PV

Contour surface of BP $s = \mathcal{L}_{\sigma^2}(h, a)$

is defined by $\mathrm{BP}_{\sigma^2}(H|y) = \text{constant for any } y \in \mathcal{B}(s)$

$\mathcal{B}(s) = \{(u, v) : v = -s(u)\}$



additivity $\mathcal{L}_{\sigma_2^2}(\mathcal{L}_{\sigma_1^2}(H, a_1), a_2) \doteq \mathcal{L}_{\sigma_1^2+\sigma_2^2}(H, a_1 + a_2)$

identity $h = \mathcal{L}_0(h, 0)$

inverse $\mathcal{L}_{\sigma^2}^{-1}(\cdot, a) \doteq \mathcal{L}_{-\sigma^2}(\cdot, -a)$

Consider contour surface of PV: $\mathrm{PV}(H|y) = \text{constant for any } y \in \mathcal{B}(s)$

then unbiasedness requires $\mathrm{BP}_1(\mathcal{R}(s)|\mu) = \text{constant for any } \mu \in \mathcal{B}(h)$

$$h = \mathcal{L}_1(s, -\lambda_0) \Rightarrow s = \mathcal{L}_{-1}(h, \lambda_0)$$

ダブルブートストラップのスケーリング則

Thm: scaling-law of DBP

$$\mathrm{DBP}_{\tau^2,\sigma^2}(H|y) \simeq 1 - \Phi\left[\beta_0\tau^{-1} - \beta_1\tau - \beta_2\tau^3 - \beta_3\tau\sigma^2\right]$$

$$\bar{\Phi}^{-1}\left[\mathrm{DBP}_{1,\sigma^2}(H|y)\right] \simeq (\beta_0 - \beta_1 - \beta_2) \underline{- \beta_3\sigma^2}$$

mean curvature of the mean curvature

平均曲率の平均曲率

$$\beta_3 = \frac{1}{2}\frac{\partial^2\gamma_1(h,u)}{\partial u_i \partial u_i}\bigg|_0$$

Corollary: DBP is third-order accurate (k=3), DAU is fourth-order accurate (k=4)

$$\mathrm{PV}(H|y) \simeq 1 - \Phi\left[\beta_0 - \beta_1 - \beta_2 + \beta_3\right]$$

$$\mathrm{DBP} = \mathrm{PV} + O(n^{-3/2}) \qquad \mathrm{DAU} = \mathrm{PV} + O(n^{-2})$$

sketch of the proof for DBP

$$s = \mathcal{L}_{\sigma^2}(h, \lambda_0)$$ contour surface of BP

$$\widetilde{\mathrm{DBP}}_{\tau^2,\sigma^2}(H|y) = 1 - \mathrm{BP}_{\tau^2}(\mathcal{R}(s)|\tilde{\mu})$$

The proof completes by applying the asymptotic expansion of BP to R(s)

棄却確率

Rejection probabilities of DBP and DAU

$$P\Big(\mathrm{DBP}_{1,\sigma^2}(H|Y) < \alpha\Big) \simeq \Phi\Big[z_\alpha - \underline{(1+\sigma^2)\beta_3}\Big]$$

mean curvature of the mean curvature

平均曲率の平均曲率

DBP is third-order accurate (k=3)

$$P\Big(\mathrm{DBP}(H|Y) < \alpha\Big) \simeq \Phi(z_\alpha - \underline{2\beta_3}) = \alpha + O(n^{-3/2})$$

DAU is fourth-order accurate (k=4)

$$P\Big(\mathrm{DAU}(H|Y) < \alpha\Big) \simeq \Phi(z_\alpha) = \alpha$$

$$\gamma_1 = \frac{1}{2}\frac{\partial^2 h(u)}{\partial u_i \partial u_i}\Big|_0$$

mean curvature of the surface

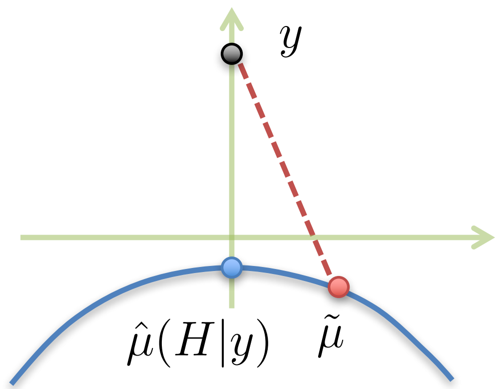
$$\beta_3 = \frac{1}{2}\frac{\partial^2 \gamma_1(h,u)}{\partial u_i \partial u_i}\Big|_0$$

mean curvature of the mean curvature

DAUは射影誤差に影響されにくい

Robustness to projection error

If $\hat{\mu}(H|y) = (0, -h(0)) \in \partial H$ is replaced by $\tilde{\mu} = (\theta, -h(\theta)) \in \partial H$



DBP becomes

$$\widetilde{\mathrm{DBP}}_{\tau^2,\sigma^2}(H|y) \simeq \bar{\Phi}\left[\beta_0\tau^{-1} - \beta_1\tau - \beta_2\tau^3 - \beta_3\tau\sigma^2 - \underline{\tau^{-1}(\tau^2+\sigma^2)\kappa(\theta)}\right]$$

error = O(n^{-1})

$$\kappa(u) = \gamma_1(h,u) - \gamma_1(h,0) - \lambda_0(\gamma_2(h,u) - \gamma_2(h,0))$$
$$\simeq (3h_{mmi} - 6\lambda_0 h_{ml}h_{mli})u_i + (6h_{mmij} - 2h_{mm}h_{li}h_{lj} - 4h_{ml}h_{mi}h_{lj})u_iu_j$$

Corollary: DBP becomes only second-order accurate (k=2), but
DAU keeps fourth-order accuracy (k=4)

$$\widetilde{\mathrm{DBP}} = \mathrm{DBP} + O(n^{-1}) \qquad \widetilde{\mathrm{DAU}} = \mathrm{DAU} + O(n^{-2})$$

Efron and Tibshirani (1998)の結果 Shimodaira (2014)

まとめ

- ブートストラップ確率はベイズ事後確率
- 頻度論のp-値との差は，仮説境界の「平均曲率」が原因
- ダブルブートストラップ法でも修正したときの誤差は，「平均曲率の平均曲率」
- マルチスケールブートストラップ法で誤差解消
- 検定以外にも使えるかも？（境界までの距離や境界の曲率を推定できる）

Summary and other issues

- DAU = "DBP with m=-n" is proposed
- The accuracy of BP is first order (k=1), AU is third-order (k=3), DBP is third-order (k=3)
- DAU is fourth-order accurate (k=4)
- DAU is robust to the projection error (surprisingly, k=4)
- Geometry of surfaces played important roles

- Shimodaira (2008) showed another theory of AU using unusual asymptotic theory of "nearly flat surfaces"

- Shimodaira (2004) discussed deviation from the multivariate normal model, and results for exponential family distributions are given there for multistep-AU

- Future topics may be DAU for nearly flat surfaces, or for exponential family distributions