WC10 発表／参加報告

株式会社　インシリコデータ
湯田　浩太郎
http://www.insilicodata.com

「QSAR」の言葉のルーツとなられた
藤田稔夫先生が８月２２日に**逝去されました**

心よりご冥福をお祈りいたします

QSAR（**Q**uantitative **S**tructure **A**ctivity **R**elationships)

Sponsors

JOHNS HOPKINS BLOOMBERG SCHOOL of PUBLIC HEALTH

Countdown

It is finally here!
Days Hr Min Sec

The 3Rs in Action

Welcome to the website of the 10th Congress on Alternatives and Animal Use in the Life Sciences. The congress will take place at the Washington State Convention Center in Seattle, Washington, USA on **August 20-24, 2017**.

We are pleased to invite you to the 10th World Congress on Alternatives and Animals in the Life Sciences (WC10), which will be held on 20-24 August 2017 in Seattle, Washington, USA. The theme for this Congress is "The Three Rs in Action."

WC10 promises to be a cutting edge scientific meeting with emphasis on the latest technologies for reduction and replacement of animals and innovations in approaches to ethics, animal welfare and public policy. Its placement in Seattle offers a broader reach to countries in Asia that are strengthening their focus on the Three Rs. The occurrence of the 10th in a series of World Congresses in the area of Alternatives and Animal Use in the Life Sciences is a milestone and correlates with the 10th anniversary of the National Research Council report on Toxicity Testing in the 21st Century – A Vision and a Strategy – a perfect occasion to take stock on our progress.

We look forward to seeing you in Seattle in 2017!

Elaine Faustman, Robert Kavlock and Joanne Zurlo, Congress Co-chairs

We look forward to seeing everyone in Seattle!

ABSTRACT BOOK NOW AVAILABLE

PROGRAM

WC 10 APP DOWNLOAD

PLENARY SPEAKERS

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☐Scientific Program Overview

Themes:

I. Ethics
II. Lessons Learned
III. Innovative Models for Safety and Efficacy
IV. Sustainability
V. Systems Biology and Big Data
VI. 3Rs in Academia
VII. Translation
VIII. Refinement and Animal Welfare
IX. Global Cooperation

Read Across 関連発表

招待講演：
Thomas Hartung; Read-Across Based QSAR for REACH

口頭発表：
II-3-431 Grace Patlewicz: Using High-Throughput Literature Mining to Support Read-Across Predictions of Skin Sensitization
IV-1-165 Anne Bonhoff: Automated Read-Across for REACH
VII-3-776 Ivan Rusyn: Read-Across and Grouping of Complex Substances Using Bioactivity Data from Human Induced Pluripotent Stem Cell (iPSC)-Derived Models
IX-3-491 Gladys Ouedraogo: Exploring the Value of New Approach Methodologies in Read-Across: The Parabens as a Collaborative EU-ToxRisk–Cosmetics Europe Case Study

Session II-5: Read Across
Co-Chairs: Grace Patlewicz, USEPA, RTP, NC, USA
Masamitsu Honma, National Institute of Health Sciences, Tokyo, Japan
II-5-432 Grace Patlewicz: Navigating Through the Minefield of Read-Across: From Research to Practical Tools
II-5-645 Sunil Kulkarni: Read-Across: Lessons Learned & Success Stories from Canada's Chemicals Management Plan
II-5-561 Takashi Yamada: Our Recent Experiences for Development of Read-across Approach for Chemical Safety Assessment
II-5-671 Francis Kruszewski: Benefits of Using Read Across and in Silico Techniques to Fill Non-SIDS Data Gaps for High Production Volume Chemical Categories
II-5-126 George Helman: Case Study of Read-across Predictions Using a Generalized Read-Across (GenRA) Approach
II-5-632 Q. Jay Zhao: Application of Read-Across in Quantitative Chemical Risk Assessment in a Regulatory Setting

ポスター発表：
・Exploring the value of new approach methodologies in read-across: the parabens as a collaborative EU ToxRisk - Cosmetics Europe case study; Ouedraogo G, Van der Burg B, Mahony C, Naciff J, Ellison C, Detroyer A, Bury A, Drewe W, Long T, Kamp7, Dinant Kroese H, Escher S, Cull T, White A, Dent M, Blaauboer B, Keller D, Willighagen E, Cronin M, Currie R, Gräpel R, Van de Water B, Mombelli E.
・Lessons from Read-Across Case Studies for Repeated-Dose Toxicity; Mahony C, Schultz TW, Cronin MTD.

In Silico 関連発表

招待講演:

Tuesday, August 22, 2017
Read-Across Based QSAR for REACH
12:15 – 13:00 Room 609
Speakers: Thomas Hartung, MD, Ph.D, The Johns Hopkins, University Bloomberg School of Public Health; Craig Rowlands, DABT Biosketch
This session will provide an update on the collaboration between UL and researchers from Johns Hopkins University on a read-across based QSAR tool for REACH. We will discuss how this in silico tool will help to minimize animal consumption and will predict toxicity to fill data gaps for the REACH registration process.

口頭発表:

II-2-445 Barbara Birk: The Effects of Active Transport in an In Silico-In Vitro Based Risk Assessment Approach for Potential Endocrine Disrupting Substances
III-15-480 Miyoung Yoon: Incorporating Metabolism into a Tiered Testing Scheme Based on the Combination of In Vitro and In Silico Approaches
III-15-701 Barbara Wetmore: Advances in In Vitro and In Silico Tools for Toxicokinetic Dose Modeling and Predictive Toxicology
5-671 Francis Kruszewski: Benefits of Using Read Across and in Silico Techniques to Fill Non-SIDS Data Gaps for High Production Volume Chemical Categories
II-6-291 Yuko Nukada: Construction of Mechanism-Based Hepatotoxicity Prediction System by Combining in Silico and In Vitro Technology
V-3-647 Glenn Myatt: The Development of in Silico Toxicology Protocols
IX-6-499 Paul Carmichael: Report on the Unilever and EPA Collaboration on Developing In Vitro and In Silico Methods for Toxicological Risk Assessment

ポスター発表:

・Paul Carmichael: Report on Unilever and EPA collaboration on developing in vitro and in silico methods for toxicological risk assessment
・Bridging the gap from external to internal exposure: use of in silico, PBPK and in vitro methods to predict the biokinetics of topically applied cosmetic ingredients; Klaric M, Cubberley R, Duplan H, Eilstein J, Ellison C, Grégoire S, Hewitt N, Jacques-Jamin C, Lange D, Roe A, Rothe H, Schepky A.

WETとDRYの融合による
新たな化合物安全性評価への可能性

プライバシー保護のため写真を省略いたします。

Moo-Yeal Lee, Ph.D.

I really want to find out a way to predict human toxicity (e.g., Cmax or true/false of toxicity in humans) from in vitro data.

省略

省略

省略

省略

3次元細胞を用いたスクリーニングデータによる毒性評価

条件１：新しいWET実験手法が日進月歩で開発・研究されている。
二次元培養細胞（従来の高速スクリーニング）から、より生体に
近いと考えられる3次元培養細胞利用による in vitro データ利用で、
in vivoデータに近い結果が期待

条件２：実験手法の開発のみならず、新たに得られるデータを
用いて、従来よりも付加価値の高い結果に導きたいが、そのデータ解析をできる環境がない。
（3次元細胞を用いたスクリーニングデータ毒性評価）

**WETとDRYの連携により、
より高い目標を実現するチャンスがある**

KY法関連のポスター発表

Development of new data analysis methods : KY-methods

Kohtaro Yuta
k-yuta@insilicodata.com
The In Silico Data Ltd., Japan

1. Preface

The KY-method is a data analysis method featuring multistep re-sampling process.

Currently 6 types of KY-method are developed. There are three types as classification methods of two classes, and three types as multiple regression methods. The KY method achieves an extremely high classification rate in the two class classification method and realizes an extremely high determination coefficient in the multiple regression method.

2. Basic composition of KY-method

In the KY-method, various existing data analysis methods are used as classification method and multiple regression method. Therefore, the KY-method is not a specific data analysis method but a "meta data analysis method" developed in combination with an existing data analysis method. For example, in the two-class classification KY-method, various data analysis methods such as SVM (Support Vector Machine), AdaBoost, NN (Neural Network), Bayesian Analysis and other various discriminant analysis methods are applied. Likewise, in the multiple regression KY-method, it is possible to apply various methods such as linear / nonlinear regression, logistic regression, PLS (Partial Least Squares), etc. in the multiple regression method.

3. Excellent feature of KY-method

The KY-method does not deteriorate the accuracy of data analysis even if a large number of samples are used. Therefore, the KY-method has a powerful and optimum function corresponding to the future big data era.

(1) Sample number free: The KY method has a feature that data analysis accuracy does not drop even if the number of samples is extremely large. This is because sample groups are classified into small groups at individual step, so that the number of samples is relatively small, which makes it possible to avoid degradation of data analysis accuracy.

(2) By the KY-method, classification accuracy and coefficient of determination can be increased: In the KY-method, noise samples are put together and transfer to the next step. For this reason, it is possible to analyze the data without noise samples within each step. As a result, data analysis can be performed without decreasing the classification rate and the determination coefficient.

(3) The KY-method is a meta analysis method to which existing methods are applied as a data analysis method applied at individual stages. This makes it easy to incorporate data analysis methods to be developed in the future, and can always work with the latest methods.

4. Types of KY-method

The KY-method currently has three types as two class classification method and also three types as multiple regression method are developed.

* Two class classification KY-method:

(a) Two model KY-method　(b) One model KY-method　(c) Model free KY-method

* Multiple regression KY-method:

(a) KY-Fitting with DA (Discriminant analysis)　(b) KY-Fitting with no DA (Discriminant analysis)　(c) Model free KY-fitting

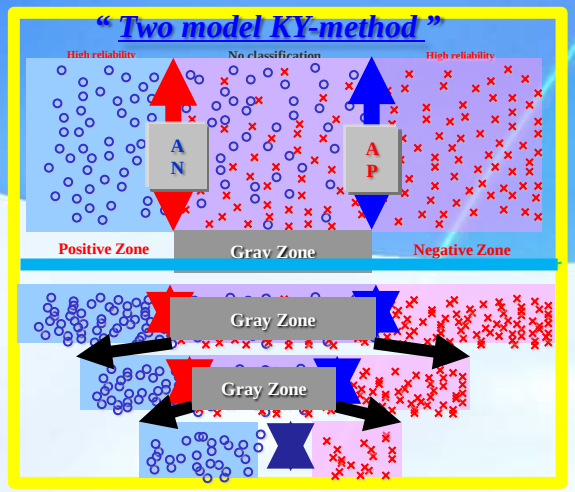
5. Summary

The KY-method is a "meta analysis method" that can improve the data analysis power possessed by the original methods. In the poster, more details on the KY-method will be discussed.

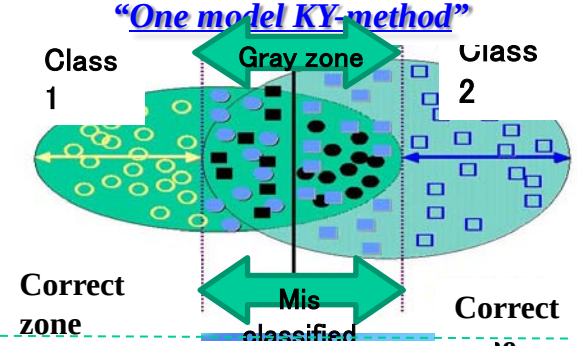
Development of new data analysis methods : The KY-methods

Kohtaro Yuta “
The In Silico Data , Ltd.
K-yuta@insilicodata.com

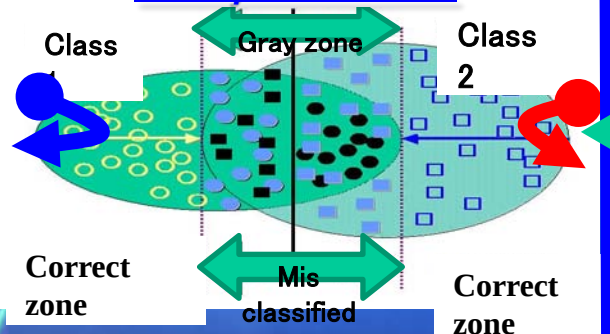
“ Two model KY-method ”



“One model KY-method”



“Model free KY-method”



◆Introduction

>Big data era has come and data analysis methods are required to handle large amounts of data.
>Now data analytical methods must handle large amounts of data and have high accuracy are required.
>The KY-methods are developed state of the art data analysis methods for which can implement the above requirements.
>By adopting the multistage iterative analysis method, the KY-method can achieve high analytical precision even when handling with a large number of samples.
>The KY-method easy to incorporate new data analysis methods which will be developed in the future.

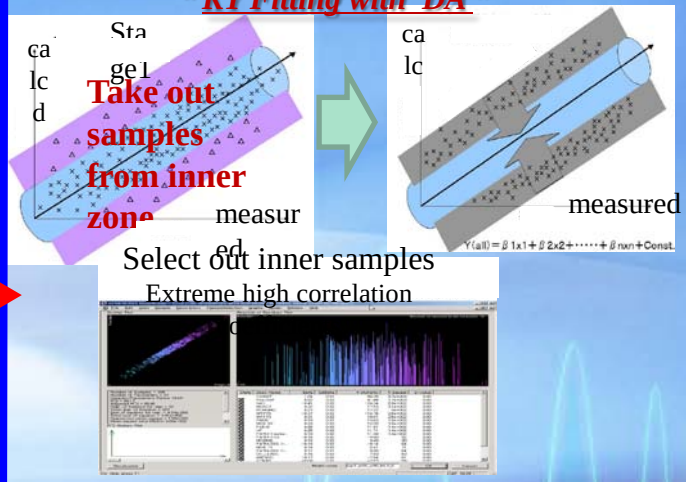
A series of the KY methods

Discriminant Analysis	Fitting
Two model KY	KY Fitting with DA
Single model KY	KY Fitting with no DA
Model free KY	Model free KY Fitting

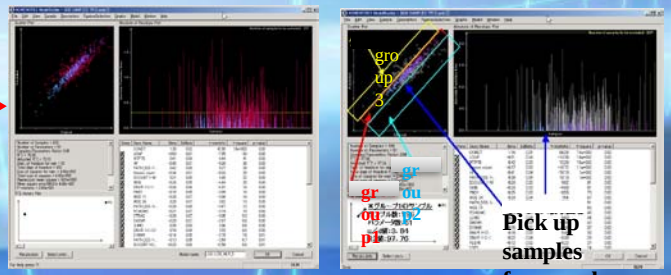
◆Conclusion

>Discriminant analysis (3 methods) and fitting (3 methods) were developed as KY-method.
>Discriminant analysis by KY-method (2 class classification) achieve 100% classification rate constantly.
> High correlation coefficient was obtained by KY fitting method.
> In the prediction rate, the model free KY-method may achieve the highest value in discriminant analysis, and the model free KY fitting is expected to achieve high value in fitting.

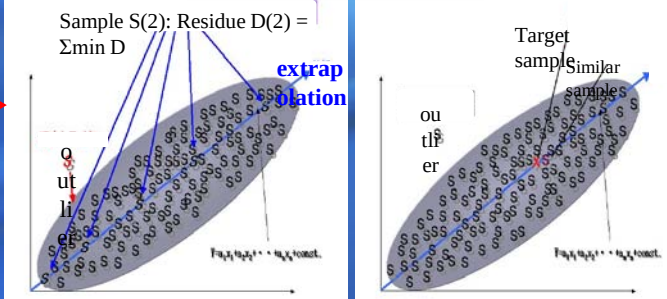
“ KY Fitting with DA ”



“ KY Fitting with no DA ”



“ Model free KY Fitting ”



□KY法の基本的特徴（データ解析能力）

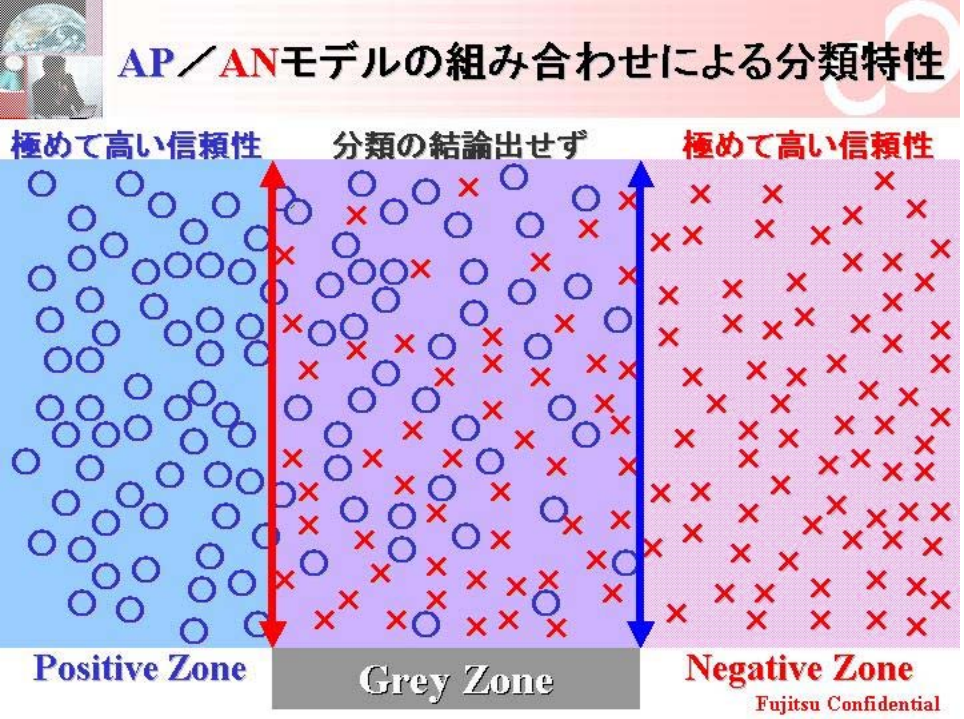
1．二クラス分類では常に100%分類実現
2．重回帰手法では極めて高い相関係数や決定係数実現

□KY法の基本的特徴（解析手順）

1．良サンプルおよびグレーサンプル選択
2．　多段階手続き

□KY法の基本的特徴（手法的特徴）

1．基本となる解析手法は通常の手法を適用：メタ解析手法
2．新たに開発される手法の取り込みが容易



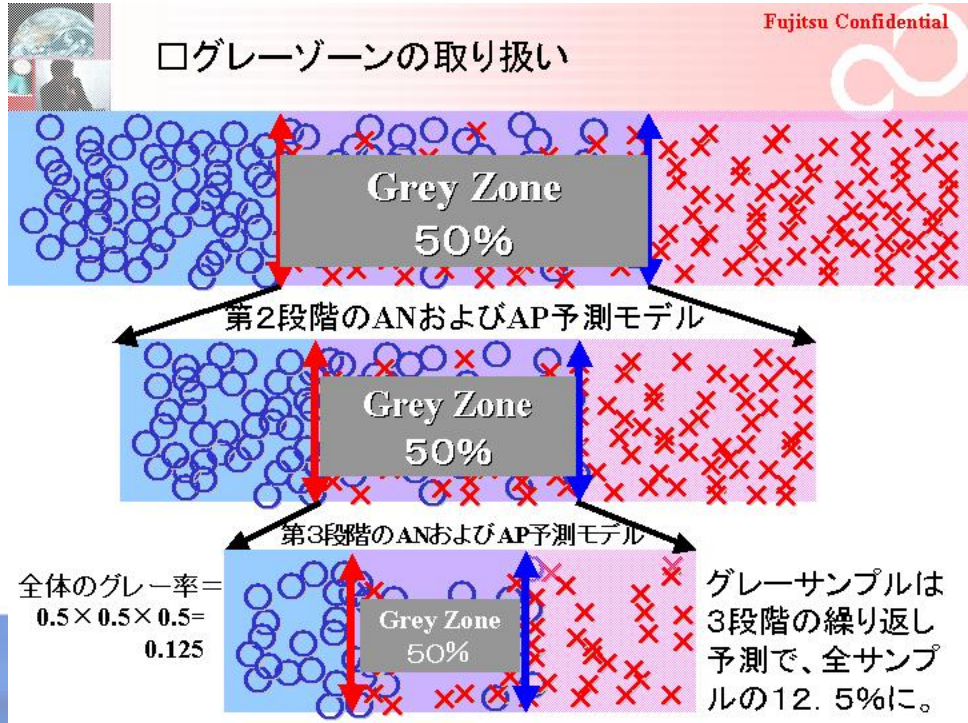
Two model KY

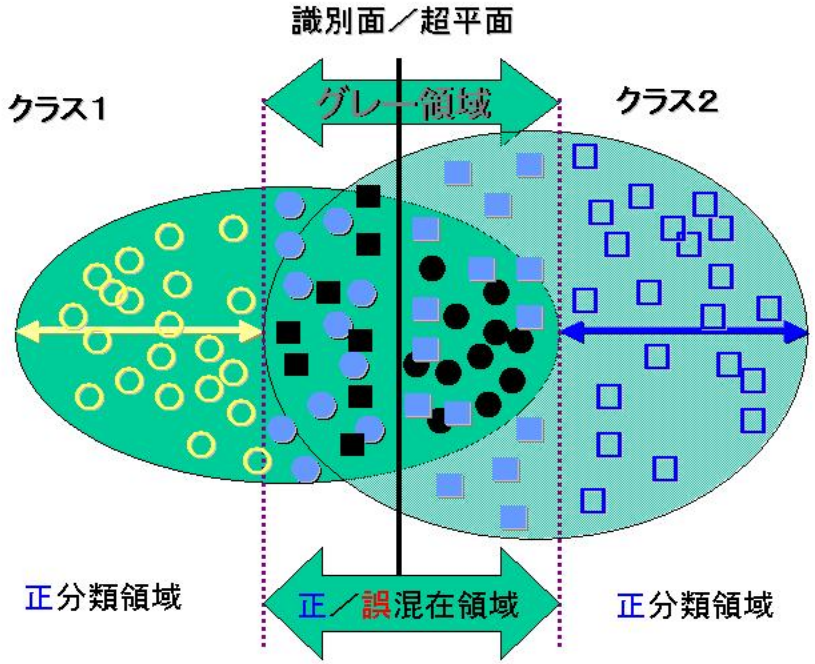
Original KY

ニクラス分類手法

KY（K-step Yard sampling）法 オリジナル

＊二本の判別関数を用いる





Single model KY

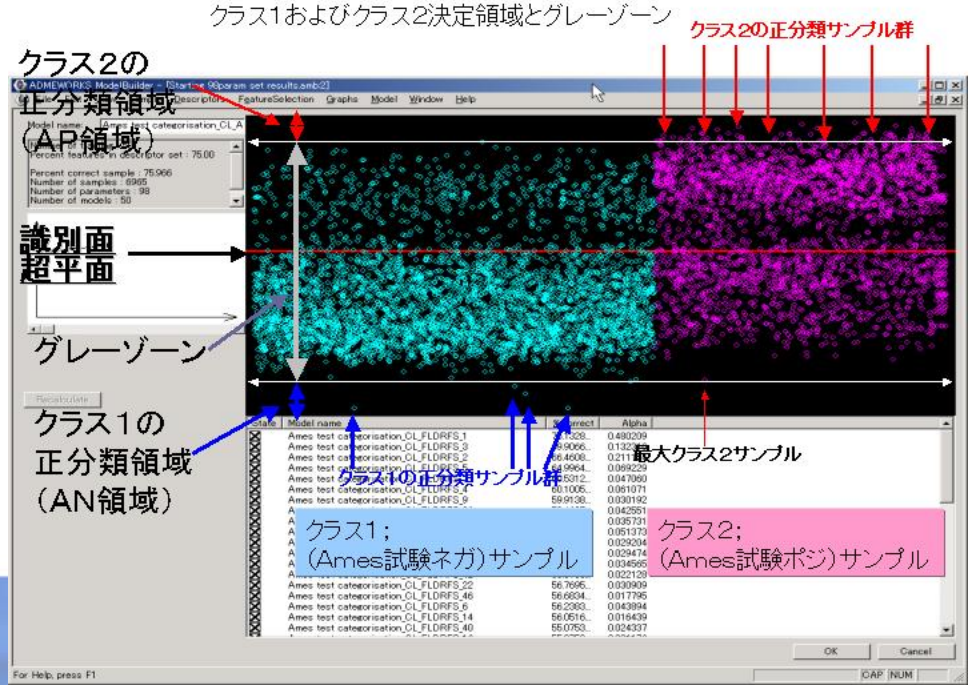
(Super KY)

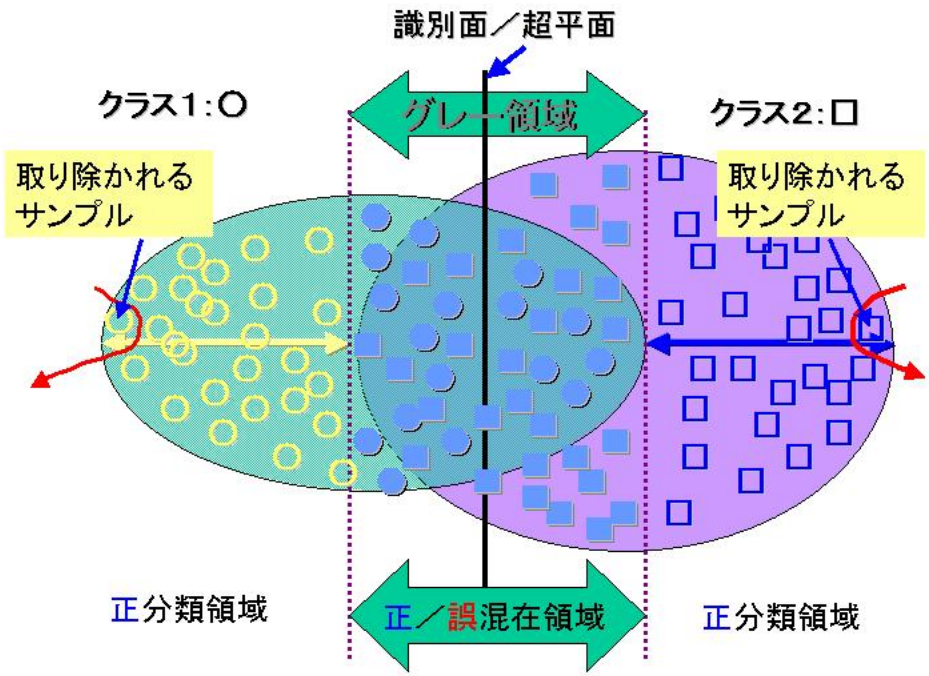
ニクラス分類手法

□手法の特徴

1. 1本の判別関数でKY法実施
2. 2モデルKY法より手順が簡単且つより高い予測性

AdaBoostを分類手法として用いた時の
クラス1およびクラス2決定領域とグレーゾーン





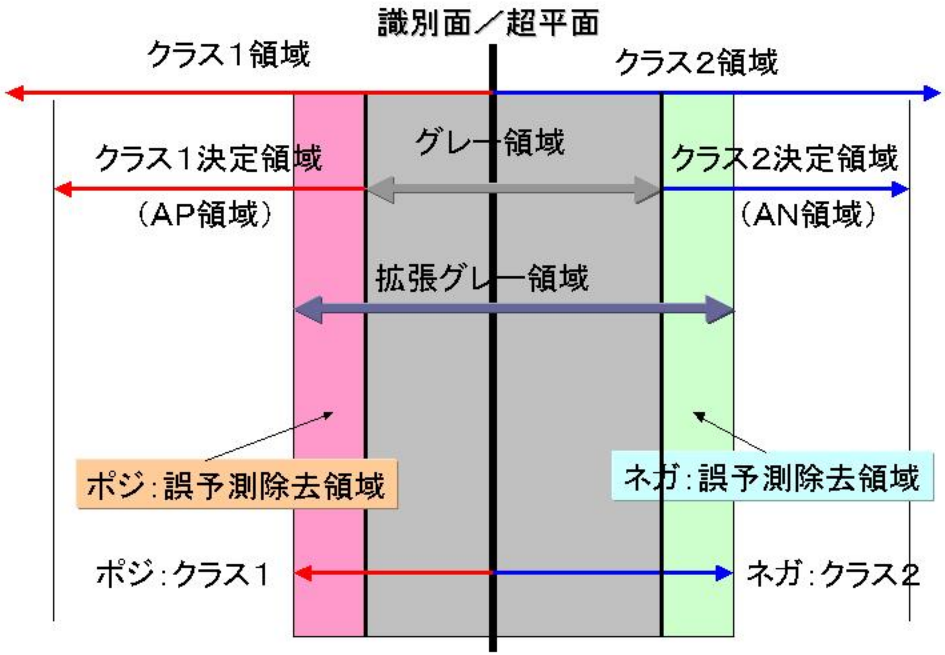
Model free KY

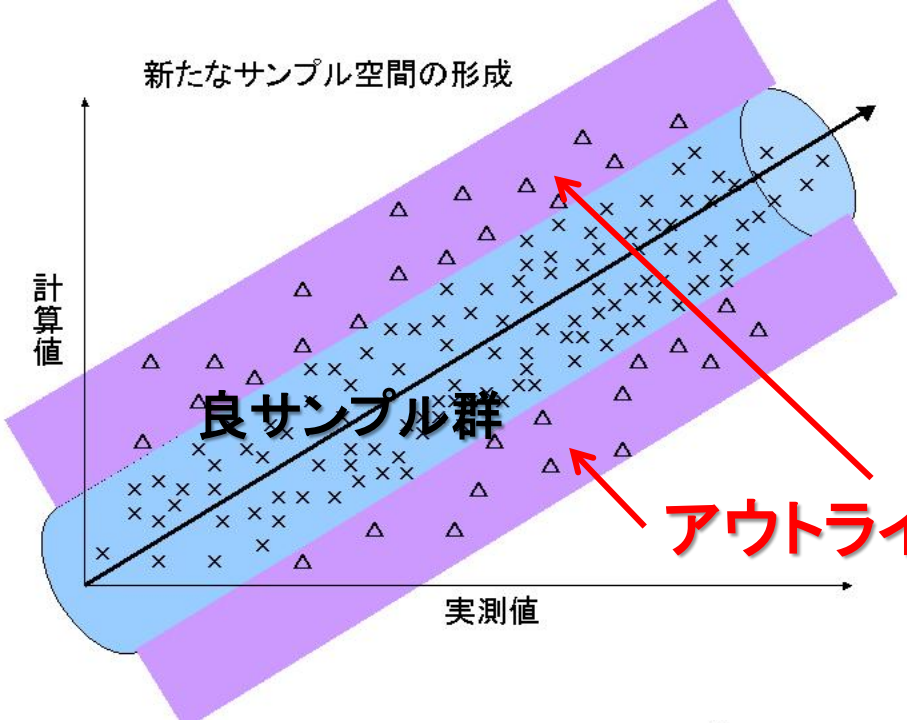
(Miracle KY)

ニクラス分類手法

□手法の特徴

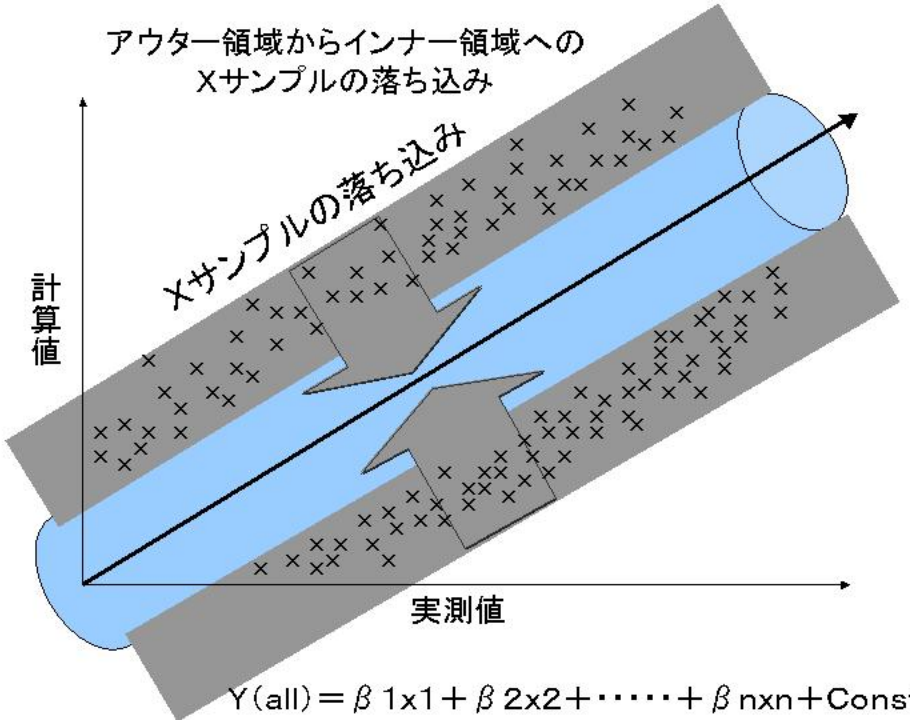
1. 判別関数を用いるが、
   分類目的ではない
2. 良好なサンプルを外部より
   順に取り出してゆく
3. 簡単且つより高い予測性
4. 自動化に適したアルゴリズム



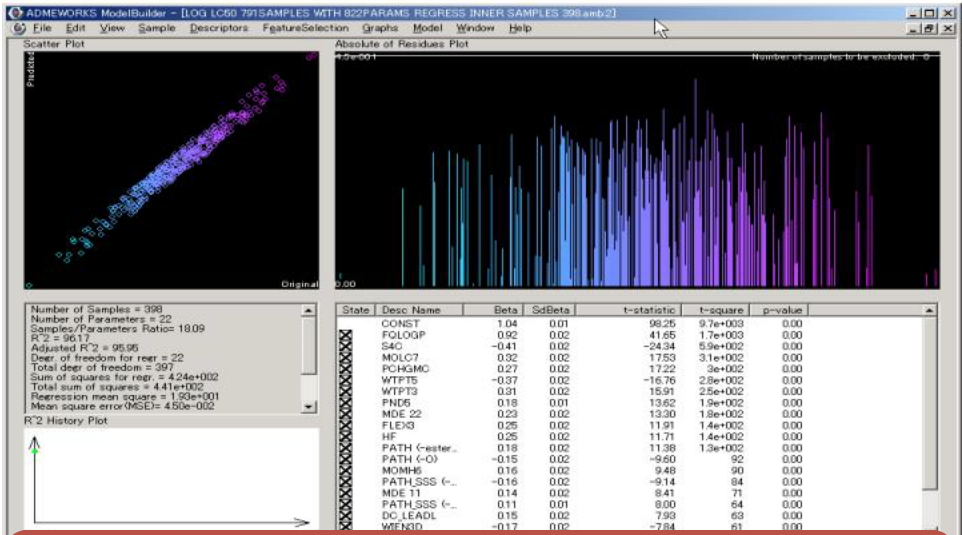


KY Fitting with DA

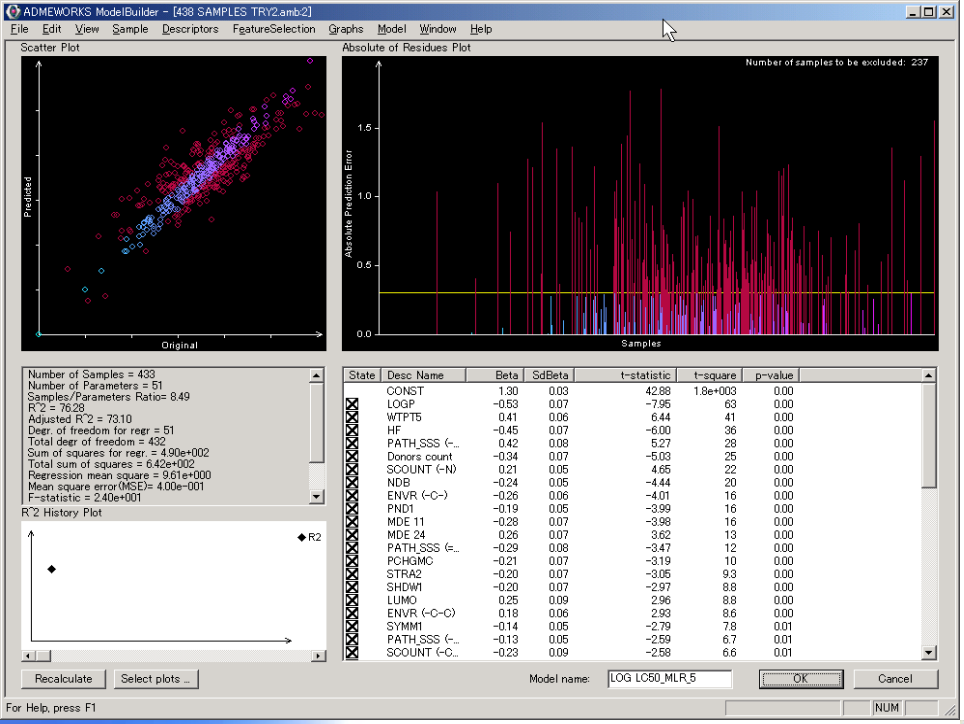
重回帰手法



ステージ1:インナーサンプル
サンプル数:398、 パラメータ数:22、 信頼性指標:18．1
R2:96．2、 R:98．1、 F値:428、 クロスバリデーション:94．4



$$Y(all) = \beta 1x1 + \beta 2x2 + \cdots\cdots + \beta nxn + Const.$$

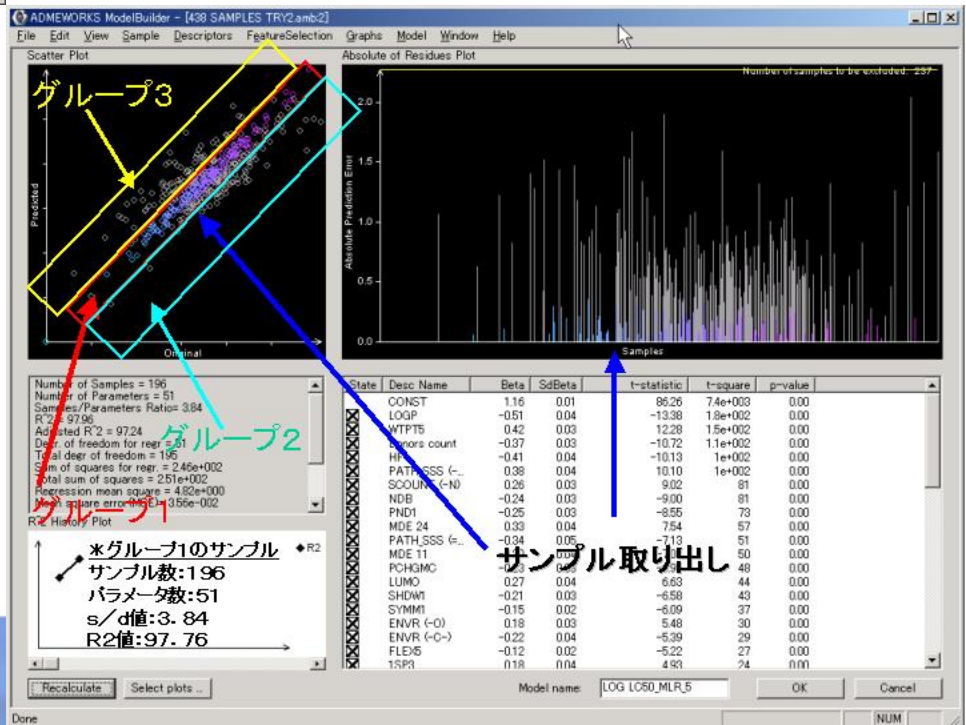


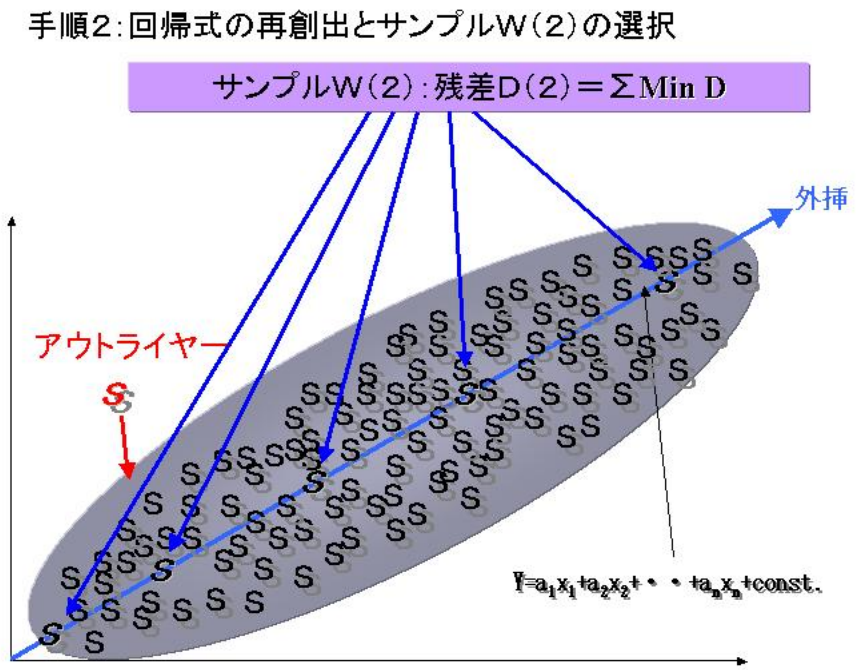
KY Fitting with no DA

重回帰手法

□手法の特徴

1. アウトライアーを残差の
　＋／－で細かく調整可能





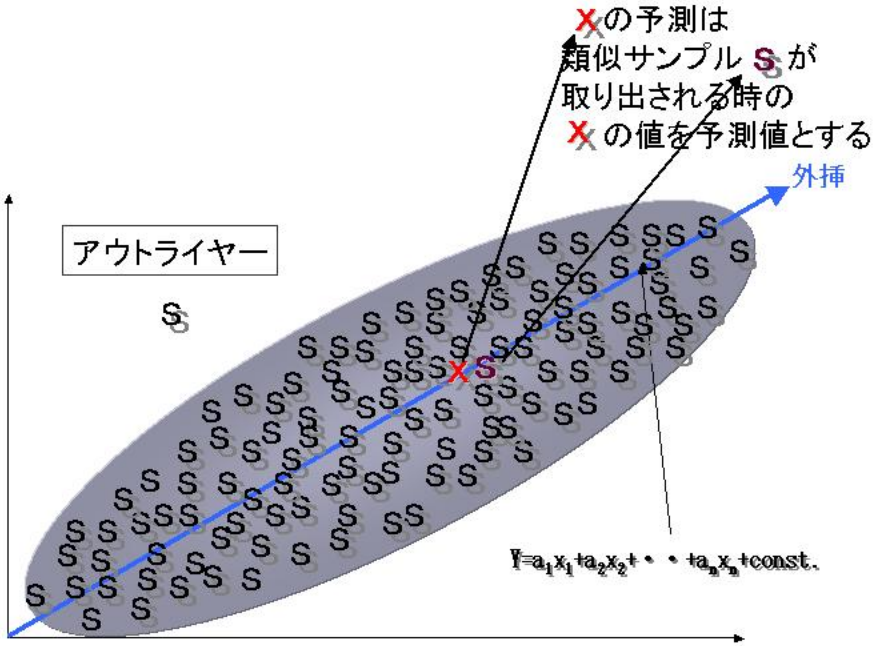
Model free

KY Fitting

重回帰手法

□手法の特徴

1. 残差が最少のサンプルから順番に取り出す
2. 残ったサンプル群で重回帰
3. 簡単且つより高い予測性
4. 自動化に適したアルゴリズム



結論：

1. KY法としての基本手続き、アルゴリズム等を確立

2. 二クラス分類に加えて重回帰への対応を実現

3. 二クラスおよび重回帰のそれぞれで3種類のKY法を展開

4. 今後は他の手法との連携等を実施し、高度な解析実現を目指す

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In Silico Data
Miracles by the KY-methods

Thank you for your attention

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