Neyman-Pearson Classification Paradigm

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Binary classification concepts and notations

- Features $X \in \mathcal{X} \subset \mathbb{R}^p$

  e.g., health characteristics of a person

- Class label $Y \in \{0, 1\}$

  e.g., disease status (YES or NO) of a person

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- A classifier is a data dependent binary function $h : \mathcal{X} \to \{0, 1\}$
- Training data $\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ (often assumed as i.i.d.)
- A classification method is a way to construct a classifier h from training data (e.g., logistic regression, support vector machines, and random forests)

  h is a function of $(X_1, Y_1), \ldots, (X_n, Y_n)$ and thus random

Classification errors

Let (X, Y) denote random variables independent of and identically distributed as (X_i, Y_i) in the training data

- Classification error ("risk")

$$\begin{aligned} R(h) &= \mathbb{P}(h(X) \neq Y) \\ &= \mathbb{P}(Y = 0) R_0(h) + \mathbb{P}(Y = 1) R_1(h), \end{aligned}$$

where

$R_0(h) = \mathbb{P}\left(h(X) \neq Y | Y = 0\right)$ denotes the type I error,
$R_1(h) = \mathbb{P}\left(h(X) \neq Y | Y = 1\right)$ denotes the type II error.

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- Randomness

  $\mathbb{P}$ w.r.t. the joint distribution of (X, Y)
  $\mathbb{P}$ w.r.t. the marginal distribution of Y
  $\mathbb{P}$ and $\mathbb{P}$ w.r.t. the conditional distribution of $X \mid (Y = 0)$ and $X \mid (Y = 1)$
  All conditional on h (i.e., conditional on the training data)

- $R(h)$, $R_0(h)$ and $R_1(h)$ are all random if h is random

Classical paradigm (theory)

- Classical goal: find a classifier h to minimize $R(h)$
- Classical oracle classifier

$$h^* = \text{argmin}_h R(h)$$

an unobservable (fixed) classifier among a class of binary functions

- Bayes classifier = classical oracle classifier

$$h^*(x) = \mathbb{I}(\eta(x) \geq 1/2)$$

where $\eta(x) = \mathbb{P}(Y = 1|X = x)$.

Classical paradigm (theory)

Classical oracle inequality

$$\mathbb{P}\left(|R(\hat{h}) - R(h^*)| \leq f(n)\right) > 1 - \delta\,,$$

where

- $\hat{h}$ is a (random) classifier trained from the training data
- h^* is the (fixed) Bayes classifier not observable
- f is a decreasing function of sample size n, $f(n) \to 0$ as $n \to \infty$
- $\delta \in (0, 1)$ is a small constant indicating the violation probability
- $1 - \delta$ is often referred to as high probability

Classical paradigm (theory)

Two approaches to construct $\hat{h}$

- Empirical risk minimization

$$\hat{h} = \text{argmin}_h \hat{R}(h)$$

where $\hat{R}(h) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{I}(h(X_i) \neq Y_i)$ is the empirical risk

- Plug in

$$h^*(x) = \mathbb{I}(\eta(x) \geq 1/2)$$
$$\eta(x) = \mathbb{P}(Y = 1|X = x) = \frac{f_1(x)\mathbb{P}(Y=1)}{f_0(x)\mathbb{P}(Y=0)+f_1(x)\mathbb{P}(Y=1)}$$
$$\hat{\eta}(x) = \widehat{\mathbb{P}}(Y = 1|X = x) = \frac{\hat{f}_1(x)\widehat{\mathbb{P}}(Y=1)}{\hat{f}_0(x)\widehat{\mathbb{P}}(Y=0)+\hat{f}_1(x)\widehat{\mathbb{P}}(Y=1)}$$

$\hat{\eta}(x)$ is constructed from the training data

$$\hat{h}(x) = \mathbb{I}(\hat{\eta}(x) \geq 1/2)$$

Motivations for asymmetric error control

Classification error ("risk")

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Example: cancer diagnosis

- Mispredicting a normal tissue sample as malignant
  $\Rightarrow$ patient anxiety & additional medical costs
- Mispredicting a tumor sample as normal
  $\Rightarrow$ life loss 😭

We need classifiers to enable asymmetric error control

Population and empirical classification errors

Let $\hat{h}$ be a classifier constructed from the training data

$$\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$$

Denote the test data as

$$\{(X_1', Y_1'), \ldots, (X_m', Y_m')\}$$

Risk

- Population

$$R(\hat{h}) = \mathbb{P}_{(X,Y)}(\hat{h}(X) \neq Y)$$

- Empirical (training)

$$\hat{R}(\hat{h}) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{I}(\hat{h}(X_i) \neq Y_i)$$

- Empirical (test)

$$\tilde{R}(\hat{h}) = \frac{1}{m} \sum_{i=1}^{m} \mathbb{I}(\hat{h}(X_i') \neq Y_i')$$

Population and empirical classification errors

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Type I error

- Population

$$R_0(\hat{h}) = \mathbb{P}_{X|(Y=0)}(\hat{h}(X) = 1)$$

- Empirical (training)

$$\hat{R}_0(\hat{h}) = \frac{\sum_{i=1}^{n} \mathbb{I}(\hat{h}(X_i) = 1)\mathbb{I}(Y_i = 0)}{\sum_{i=1}^{n} \mathbb{I}(Y_i = 0)}$$

- Empirical (test)

$$\tilde{R}_0(\hat{h}) = \frac{\sum_{i=1}^{m} \mathbb{I}(\hat{h}(X_i') = 1)\mathbb{I}(Y_i' = 0)}{\sum_{i=1}^{m} \mathbb{I}(Y_i' = 0)}$$

Population and empirical classification errors

Let $\hat{h}$ be a classifier constructed from the training data

$$\{(X_1, Y_1), \ldots, (X_n, Y_n)\}$$

Denote the test data as

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Type II error

- Population

$$R_1(\hat{h}) = \mathbb{P}_{X|(Y=1)}(\hat{h}(X) = 0)$$

- Empirical (training)

$$\hat{R}_1(\hat{h}) = \frac{\sum_{i=1}^{n} \mathbb{I}(\hat{h}(X_i) = 0)\mathbb{I}(Y_i = 1)}{\sum_{i=1}^{n} \mathbb{I}(Y_i = 1)}$$

- Empirical (test)

$$\tilde{R}_1(\hat{h}) = \frac{\sum_{i=1}^{m} \mathbb{I}(\hat{h}(X_i') = 0)\mathbb{I}(Y_i' = 1)}{\sum_{i=1}^{m} \mathbb{I}(Y_i' = 1)}$$

How to control population type I error under α?

Suppose that a user would like to construct a classifier $\hat{h}$ with population type I error $R_0(\hat{h})$ no more than α (e.g., 0.05) with at least probability $(1-\delta)$ (e.g., 0.95). How to achieve it?

Statistical formulation

Given $\alpha, \delta \in [0,1]$, find $\hat{h}$ such that

$$\mathbb{P}\left(R_0(\hat{h}) \leq \alpha\right) > 1-\delta$$

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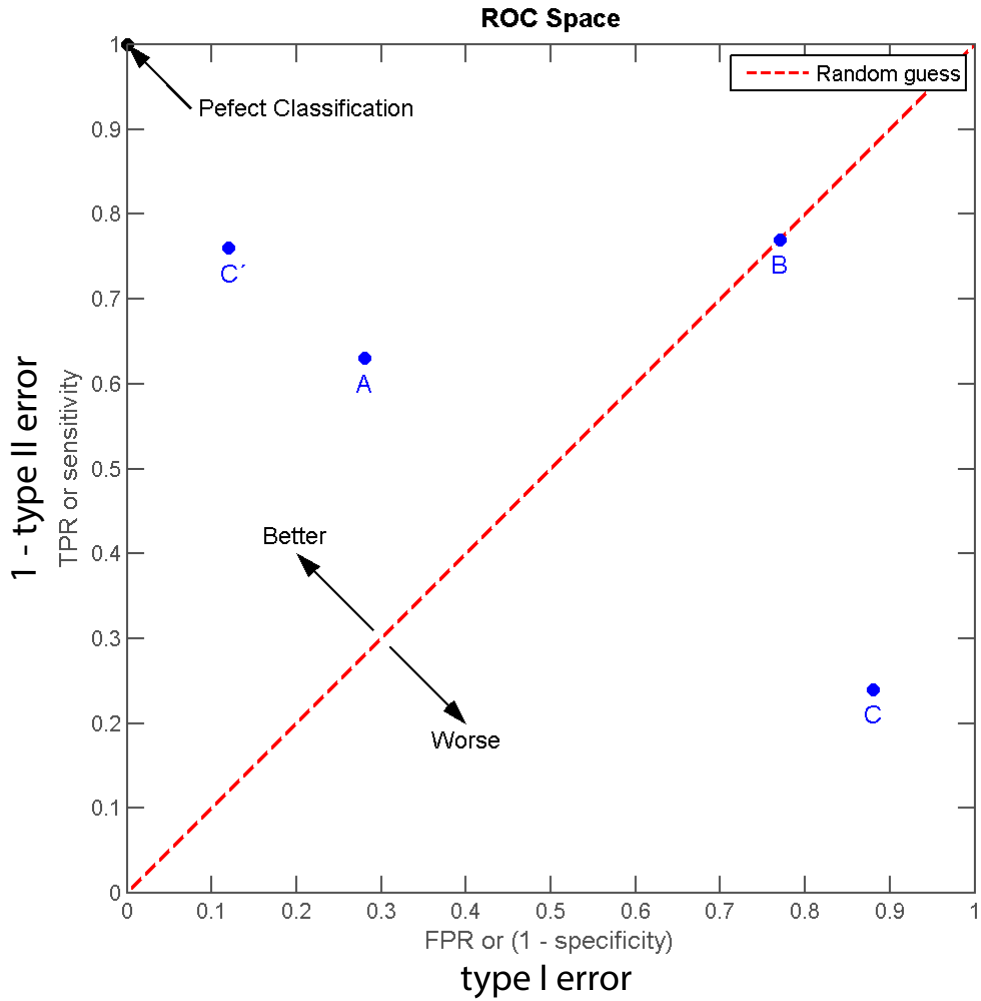
Existing approaches for asymmetric error control

- Cost-sensitive learning (Elkan, 2001; Zadrozny et al, 2003)
  - no consensus way to assign costs
  - cannot directly control the population type I error
- Receiver operating characteristics (ROC)?

Receiver operating characteristics (ROC)



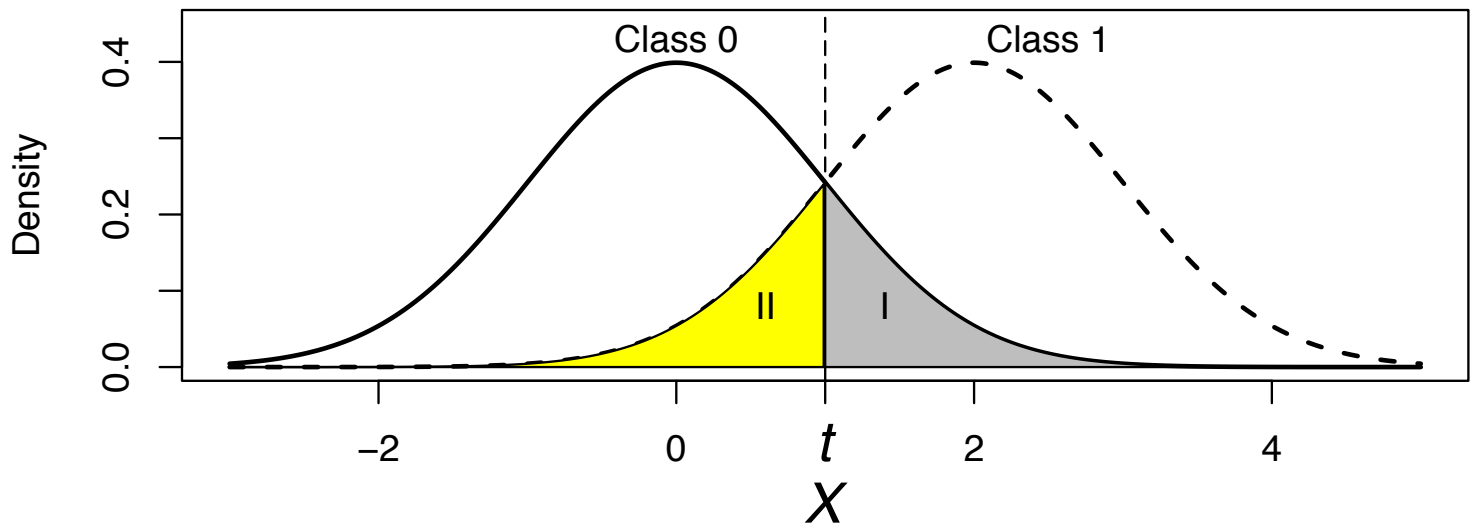
from Wikipedia

- However, ROC curves are plotted based on empirical type I and II errors in practice.

A toy example

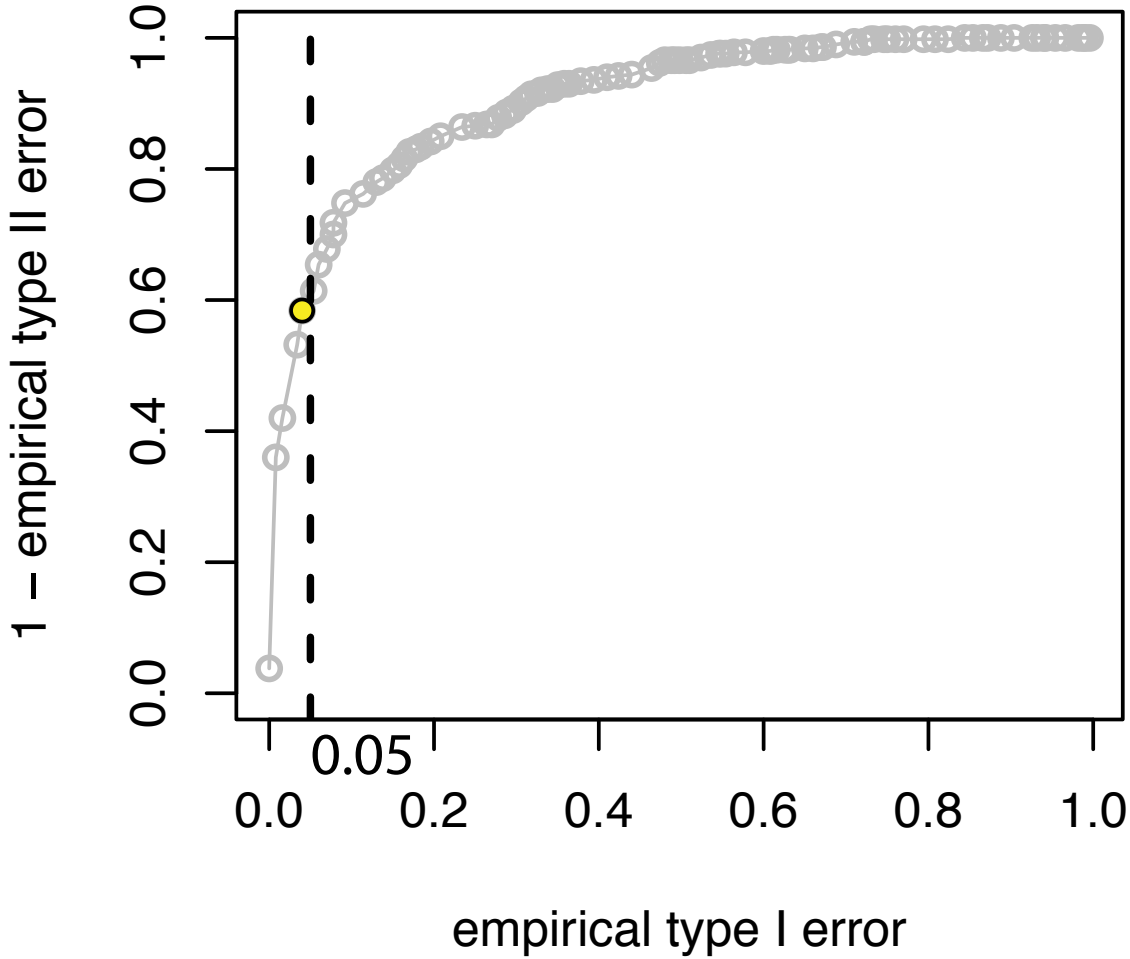
- $X|(Y=0) \sim N(0,1)$
- $X|(Y=1) \sim N(2,1)$
- $\mathbb{P}(Y=0) = 1/2$
- Classifier: $\mathbb{1}(X > t)$
- Type I error $= 1 - \Phi(t)$
- Type II error $= \Phi(t-2)$

- Training sample size $= 1,000$
- Test sample size $= 1,000$
- # of simulations $= 1,000$



Empirical type I error control != population type I error control

Data set 1



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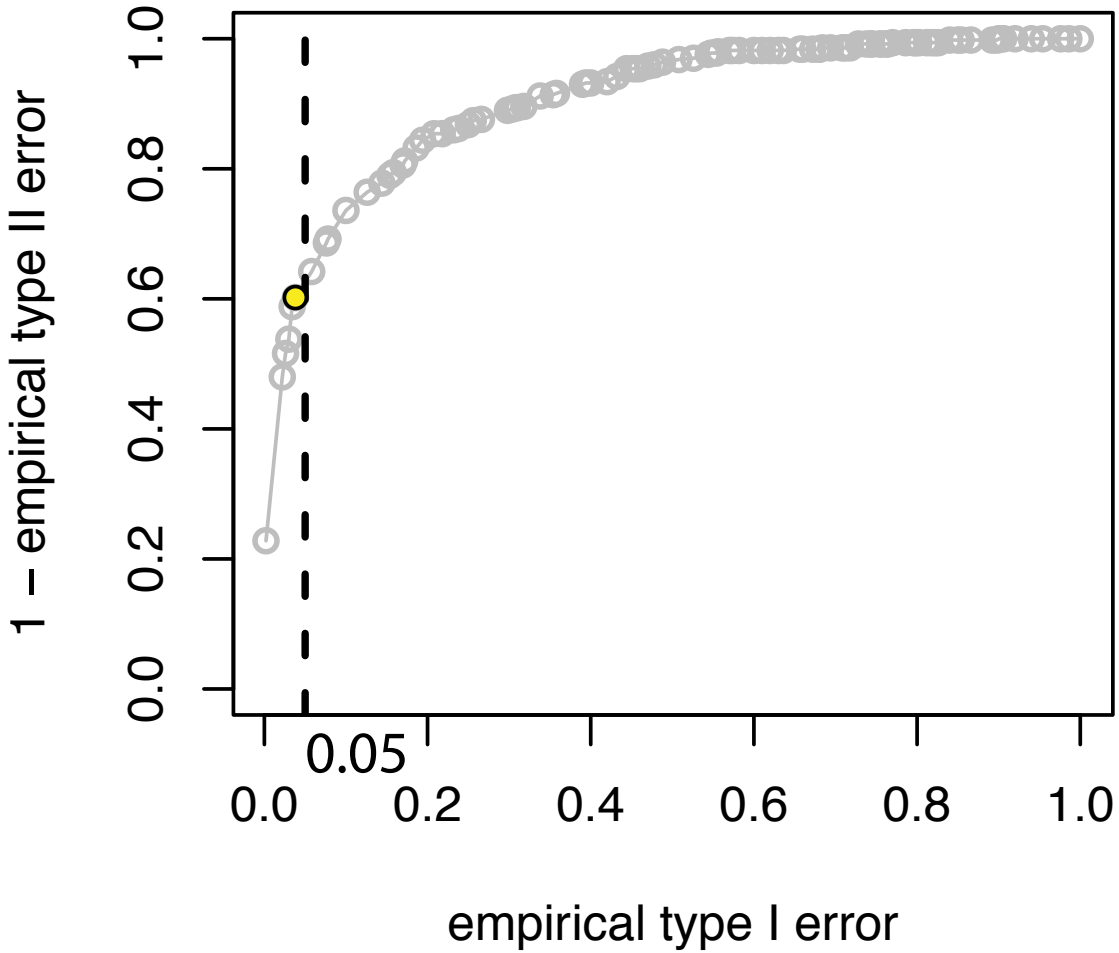
Data set 2



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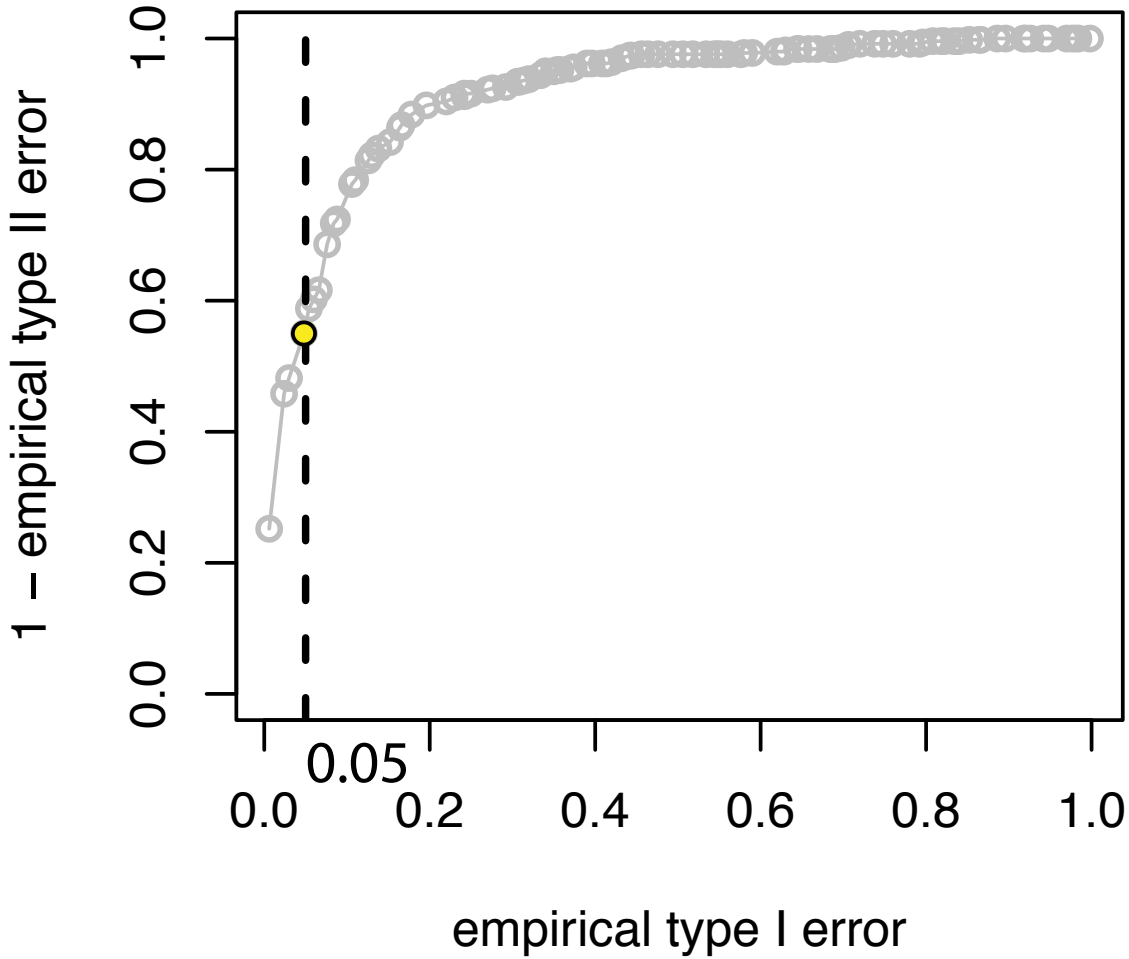
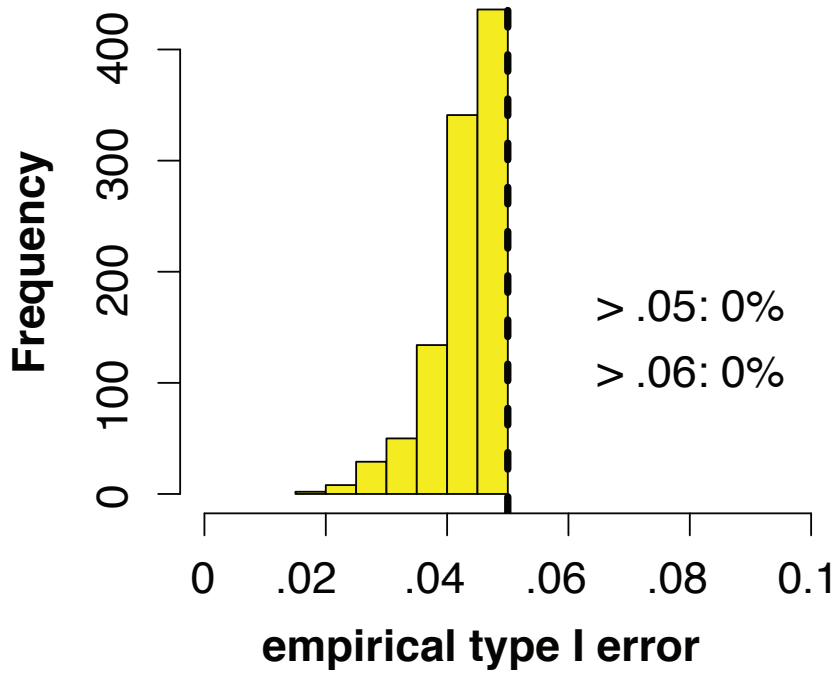
Data set $1,000$



Empirical type I error control != population type I error control

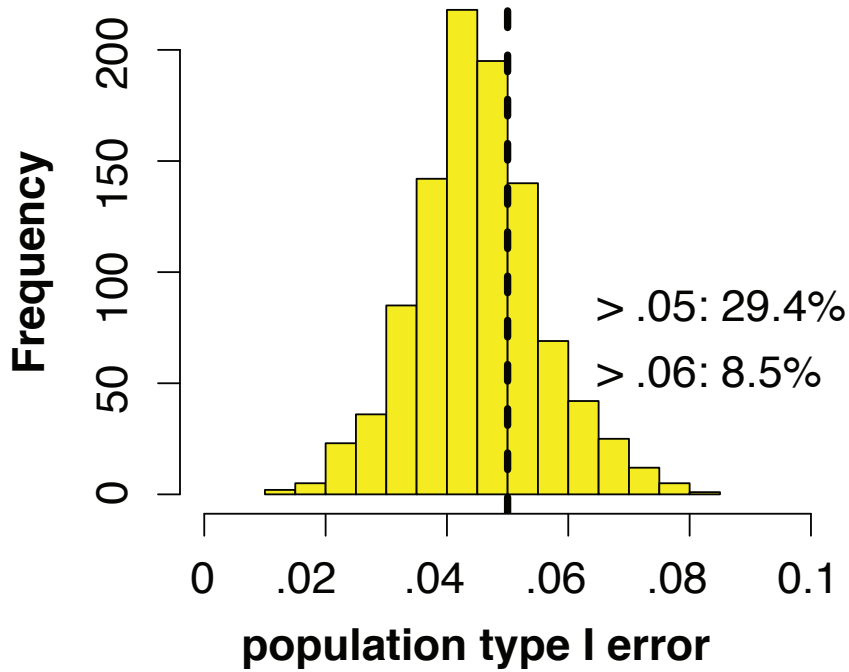
Distribution of the $1,000$ classifiers' empirical type I errors



Empirical type I error controlled? YES

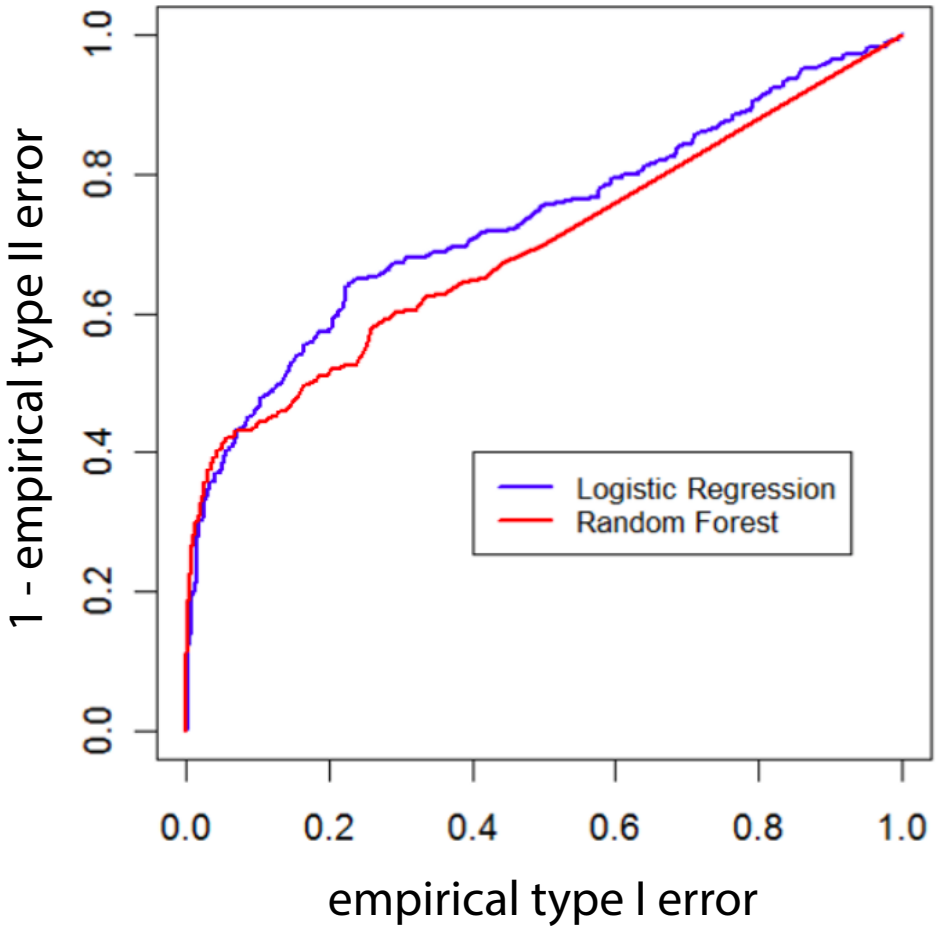
Empirical type I error control != population type I error control

Distribution of the $1,000$ classifiers' population type I errors



Population type I error controlled? NO

Choosing classifiers with population type I error control?



The empirical ROC space provides NO direct information on the population type I error control.

Neyman-Pearson Classification

The Neyman-Pearson (NP) classification paradigm

The NP paradigm seeks a classifier that satisfies:

$$\min_{R_0(h) \leq \alpha} R_1(h)\,,$$

where α is a user-specified level, usually a small value (e.g., 5%).

- Early work in the engineering community: Cannon et.al. (2002); Scott (2005)
- Our work on NP classification:
  - Rigollet and Tong (2011) (NP oracle inequalities)
  - Tong (2013) (plug-in approach)
  - Zhao et al. (2016c) (high-dimensional setting)
  - Tong et al. (2016a) (review paper)
  - Li and Tong (2016b) (genomic applications)

The Neyman-Pearson (NP) classification paradigm

Binary classification

Paradigm	Oracle classifier
Classical	$h^* = \arg\min R(h)$
Neyman-Pearson	$\phi^* = \arg\min_{R_0(\phi) \leq \alpha} R_1(\phi)$

where α reflects users' conservative attitude towards the type I error.

Neyman-Pearson (NP) oracle inequalities

- Rigollet and Tong (2011):
  Under the NP paradigm, a good classifier $\hat{\phi}$ should respect α instead of $\alpha + \epsilon$.

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  Under the NP paradigm, a good classifier $\hat{\phi}$ should respect α instead of $\alpha + \epsilon$.
- **NP oracle inequalities**: two theoretical properties should be both satisfied with high probability,
  1) $R_0(\hat{\phi}) \leq \alpha$, i.e., the type I error constraint is respected
  2) $R_1(\hat{\phi}) - R_1(\phi^*) \to 0$, i.e., the excess type II error diminishes with explicit rates (w.r.t. sample size n).

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Counterpart of

- Oracle inequality of classifier $\hat{h}$ in the classical paradigm:
  $R(\hat{h}) - R(h^*) \to 0$, i.e., the excess risk diminishes with explicit rates with high probability,

  where $h^*(x) = \mathbb{1}(\eta(x) \geq 1/2)$ is the oracle (Bayes) classifier,
  in which $\eta(x) = \mathbb{E}[Y|X = x] = \mathbb{P}(Y = 1|X = x)$ is the *regression function* of Y on X.

Connection with hypothesis testing

- The Neyman-Pearson paradigm in hypothesis testing:

  Choose ϕ to maximize $\mathbb{E}[\phi(X)|Y=1]$, s.t. $\mathbb{E}[\phi(X)|Y=0] \leq \alpha$,

  where $\alpha \in (0,1)$ is the significance level of the test.

Connection with hypothesis testing

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Neyman-Pearson Lemma

Let $\mathbb{P}_0$ and $\mathbb{P}_1$ be probability distributions possessing densities p_0 and p_1 corresponding to Classes 0 and 1. Let C_α be a density ratio threshold such that

$$\mathbb{P}_0(p_1/p_0(X) > C_\alpha) \leq \alpha \text{ and } \mathbb{P}_0(p_1/p_0(X) \geq C_\alpha) \geq \alpha.$$

Then for a given level α, the most powerful test of level α is defined by

$$\phi^*(X) = \begin{cases} 1 & \text{if} \quad p_1/p_0(X) > C_\alpha \\ 0 & \text{if} \quad p_1/p_0(X) < C_\alpha \\ \frac{\alpha - P_0(p_1/p_0(X) > C_\alpha)}{P_0(p_1/p_0(X) = C_\alpha)} & \text{if} \quad p_1/p_0(X) = C_\alpha \end{cases}$$

An NP umbrella algorithm

Adapting popular algorithms to the NP paradigm

For scoring-type classifiers (e.g., logistic regression), a classifier is constructed from

- A scoring function $f(x)$ (e.g., $f(x) = \hat{\mathbb{P}}(Y = 1|X = x)$)
- A threshold t (e.g., $1/2$)

The classifier is

$$h(x) = \mathbb{1}(f(x) \geq t)$$

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- Under the classical paradigm, only f needs to be constructed from the training data
- Under the NP paradigm, both f and t needs to be constructed from the training data given α and δ

Adapting popular algorithms to the NP paradigm

Statistical formulation

Given $\alpha, \delta \in [0, 1]$, find $\hat{h}$ such that

$$\mathbb{P}\left(R_0(\hat{h}) > \alpha\right) \leq \delta$$

- Sample splitting: split training data into two parts

  mixed classes 0 and 1 sample $\overset{\text{base algorithm}}{\Longrightarrow}$ trained scoring function

  left-out class 0 sample $\overset{\text{scoring function}}{\Longrightarrow}$ classification scores

- Threshold search: choose the smallest threshold on the classification scores such that the violation rate (i.e., the probability that the population type I error exceeds α) $\leq \delta$.
- Order statistic: find the threshold from ordered classification scores

Theoretical foundation

Lemma 1

Let $T_1, T_2, \cdots, T_n$ be independently and identically distributed (i.i.d.) real-valued random variables following a cumulative distribution function (cdf) F. Denote by $T_{(k)}$ the k-th order statistic (i.e., $T_{(1)} \leq \cdots \leq T_{(n)}$). For any t in the domain of T_i, we have

$$\mathbb{P}\left[T_{(k)} > t\right] = \sum_{i=n-k+1}^{n} \binom{n}{i} \left[1 - F(t)\right]^i \left[F(t)\right]^{n-i} .$$

- **Remark:** Lemma 1 does not have any assumptions on F. Letting $t = F^{-1}(1-\alpha)$, we derive Lemma 2 from Lemma 1.

Theoretical foundation

Lemma 2

In the same settings as in Lemma 1,

$$\mathbb{P}\left[T_{(k)} < F^{-1}(1-\alpha)\right] \;\leq\; \sum_{j=k}^{n} \binom{n}{j} (1-\alpha)^j \alpha^{n-j}\,,$$

where the equality holds for continuous F.

- **Remark:** Lemma 2 leads to the following proposition.

Theoretical foundation

Proposition

Applying a trained classification scoring function to the left-out class 0 sample (with size n), we denote the resulting classification scores as $T_1, \cdots, T_n$, which are real-valued random variables. Then we denote by $T_{(k)}$ the k-th order statistic (i.e., $T_{(1)} \leq \cdots \leq T_{(n)}$). For a new observation, if we denote its classification score, calculated by the trained base algorithm, as T, we can then construct a classifier $\hat{\phi}_k = \mathbb{I}(T > T_{(k)})$. Then the population type I error of $\hat{\phi}_k$ is

$$R_0(\hat{\phi}_k) = \mathbb{P}\left[T > T_{(k)} | T_{(k)}\right] = 1 - F(T_{(k)}).$$

Assuming that $T_1, \cdots, T_n$ are independently and identically distributed (i.i.d.), we have

$$\mathbb{P}\left[R_0(\hat{\phi}_k) > \alpha\right] \leq \sum_{j=k}^{n} \binom{n}{j} (1-\alpha)^j \alpha^{n-j}.$$

Theoretical foundation

- **Remark 1:** The probability that the type I error of $\hat{\phi}_k$ exceeds α is under a constant that only depends on k and α. We call this probability $\mathbb{P}\left[R_0(\hat{\phi}_k) > \alpha\right]$ the violation rate of $\hat{\phi}_k$, and denote its upper bound by

$$v(k) = \sum_{j=k}^{n} \binom{n}{j} (1-\alpha)^j \alpha^{n-j}.$$

  When T_i's are continuous, this bound is tight.

Theoretical foundation

- **Remark 2:** To minimize the type II error, the optimal order should be

$$k^* = \min \{k \in \{1, \cdots, n\} : v(k) \leq \delta\} \ .$$

- **Remark 3:** Minimal sample size to guarantee that $\exists k$ s.t. $v(k) \leq \delta$:

$$n \geq \log \delta / \log(1 - \alpha).$$

The NP umbrella algorithm

Algorithm An NP umbrella algorithm

input:

training data: a mixed i.i.d. sample $\mathcal{S} = \mathcal{S}^0 \cup \mathcal{S}^1$, where $\mathcal{S}^0$ and $\mathcal{S}^1$ are class 0 and class 1 samples respectively

α: type I error upper bound, $0 \leq \alpha \leq 1$; [default $\alpha = 0.05$]

δ: a small tolerance level, $0 < \delta < 1$; [default $\delta = 0.05$]

M: number of $\mathcal{S}^0$ random splits; [default $M = 1$]

function RANKTHRESHOLD(n, α, δ)

  for k in $\{1, \ldots, n\}$ **do** ▷ *for each rank threshold candidate* k

    $v(k) \leftarrow \sum_{j=k}^{n} \binom{n}{j} (1-\alpha)^j \alpha^{n-j}$ ▷ *calculate the violation rate with threshold* k

  $k^* \leftarrow \min \{k \in \{1, \ldots, n\} : v(k) \leq \delta\}$ ▷ *pick the minimal threshold whose violation rate is under* δ

  return k^*

The NP umbrella algorithm (cont'd)

procedure NPCLASSIFIER($\mathcal{S}, \alpha, \delta, M$)

  $n = \lceil |\mathcal{S}^0|/2 \rceil$ ▷ *denote half of the size of* $|\mathcal{S}^0|$ *as* n

  $k^* \leftarrow$RANKTHRESHOLD(n, α, δ) ▷ *find the rank threshold*

  for i in $\{1, \ldots, M\}$ **do** ▷ *randomly split* $\mathcal{S}^0$ *for* M *times*

    $\mathcal{S}^0_{i,1}, \mathcal{S}^0_{i,2} \leftarrow$ random split on $\mathcal{S}^0$ ▷ *each time randomly split* $\mathcal{S}^0$ *into two halves with equal sizes*

    $\mathcal{S}_i \leftarrow \mathcal{S}^0_{i,1} \cup \mathcal{S}^1$ ▷ *combine* $\mathcal{S}^0_{i,1}$ *and* $\mathcal{S}^1$

    $\mathcal{S}^0_{i,2} = \{x_1, \ldots, x_n\}$ ▷ *write* $\mathcal{S}^0_{i,2}$ *as a set of* n *data points*

    $f_i \leftarrow$ `classification algorithm`$(\mathcal{S}_i)$ ▷ *train a classification scoring function* f_i *by inputting* $\mathcal{S}_i$ *into the classification algorithm; let* f_i *output a larger expected value for class* 1 *data*

    $\mathcal{T}_i = \{t_{i,1}, \ldots, t_{i,n}\} \leftarrow \{f_i(x_1), \ldots, f_i(x_n)\}$ ▷ *apply the scoring function* f_i *to* $\mathcal{S}^0_{i,2}$ *to obtain a set of score threshold candidates*

    $\{t_{i,(1)}, \ldots, t_{i,(n)}\} \leftarrow sort(\mathcal{T}_i)$ ▷ *sort elements of* $\mathcal{T}_i$ *in an increasing order*

    $t_i^* \leftarrow t_{i,(k^*)}$ ▷ *find the score threshold corresponding to the chosen rank threshold* k^*

    $\phi_i(X) = \mathbb{1}\left(f_i(X) > t_i^*\right)$ ▷ *construct an NP classifier based on the scoring function* f_i *and the threshold* t_i^*

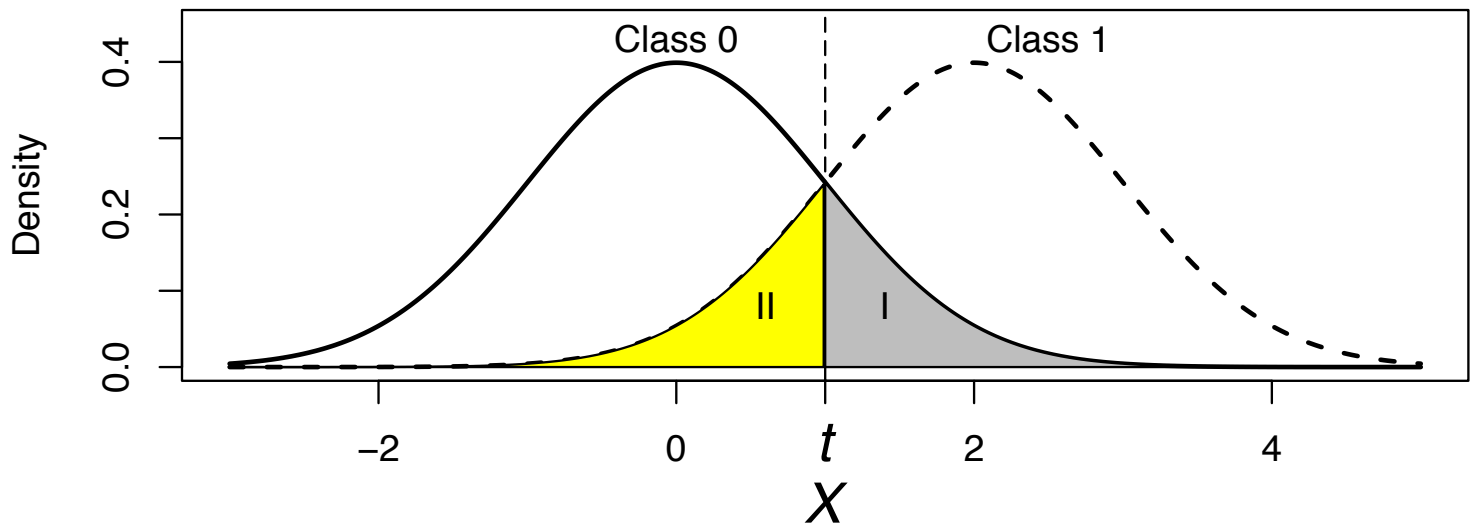
output:

  an ensemble NP classifier $\phi(X) = \mathbb{1}\left(\frac{1}{M}\sum_{i=1}^{M}\phi_i(X) \geq 1/2\right)$ ▷ *by majority vote*

Back to the toy example

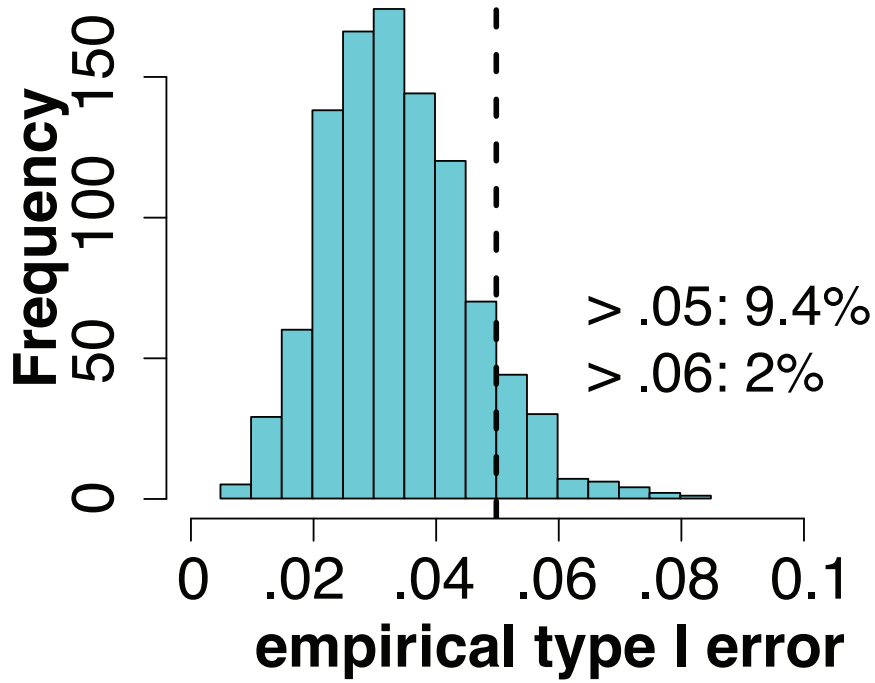
- $X|Y=0 \sim N(0,1)$
- $X|Y=1 \sim N(2,1)$
- $\mathbb{P}(Y=0)=1/2$
- Classifier: $\mathbb{1}(X>t)$
- Type I error $=1-\Phi(t)$
- Type II error $=\Phi(t-2)$

- Training sample size $=1,000$
- Test sample size $=1,000$
- # of simulations $=1,000$



NP Classifier in the toy example

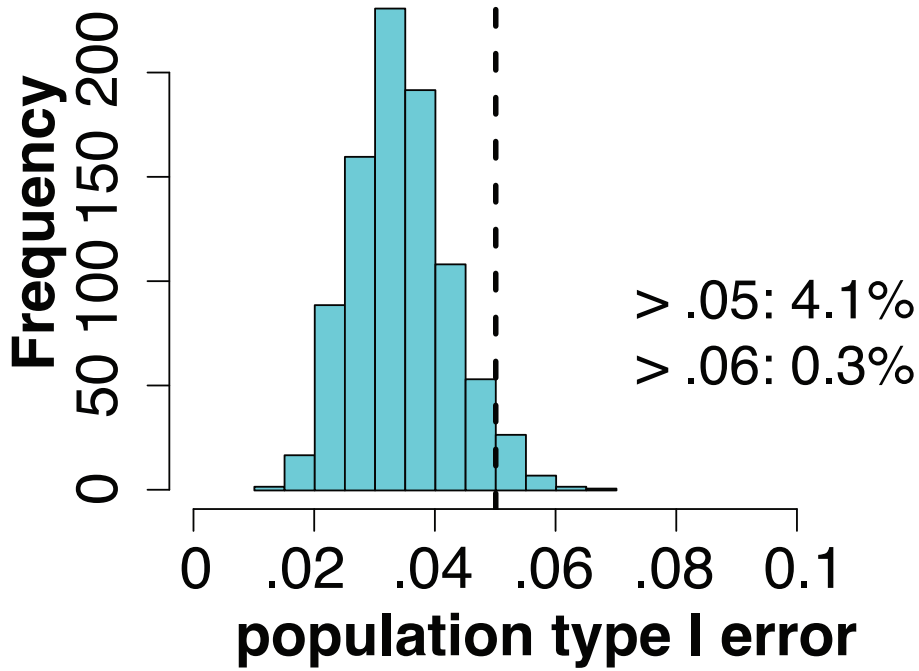
Distribution of the $1,000$ classifiers' empirical type I errors



Empirical type I error controlled? NO/YES

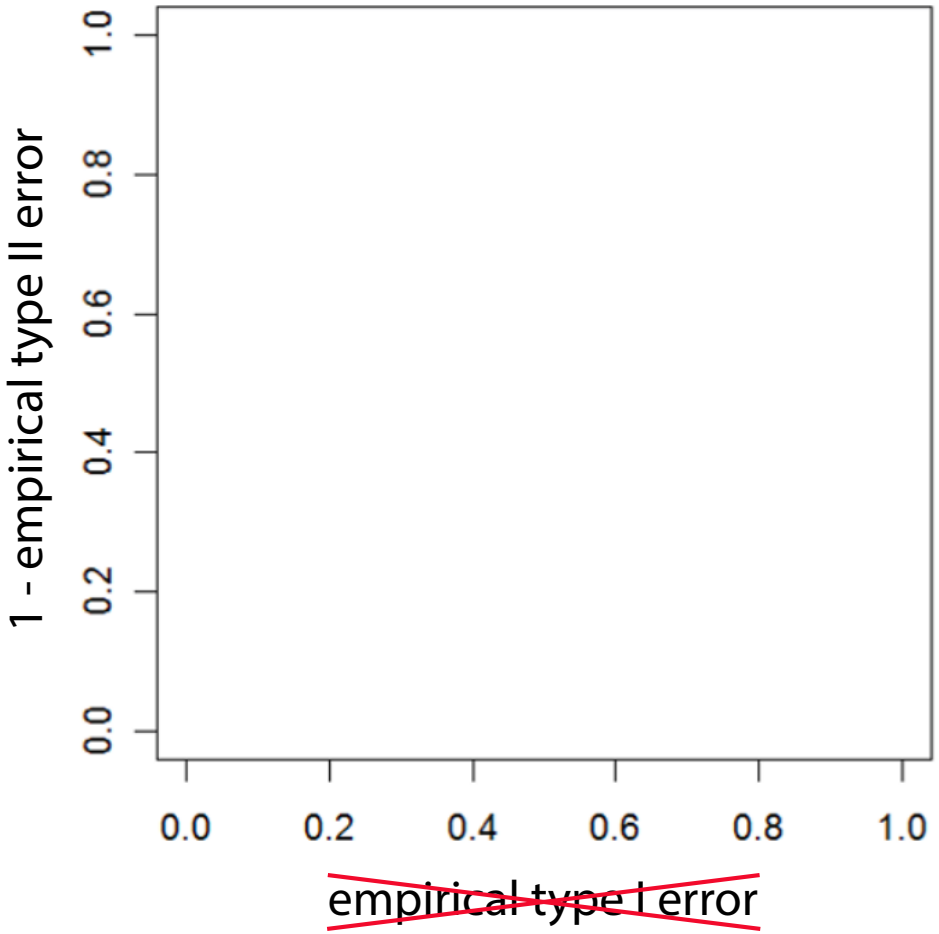
NP Classifier in the toy example

Distribution of the $1,000$ classifiers' population type I errors



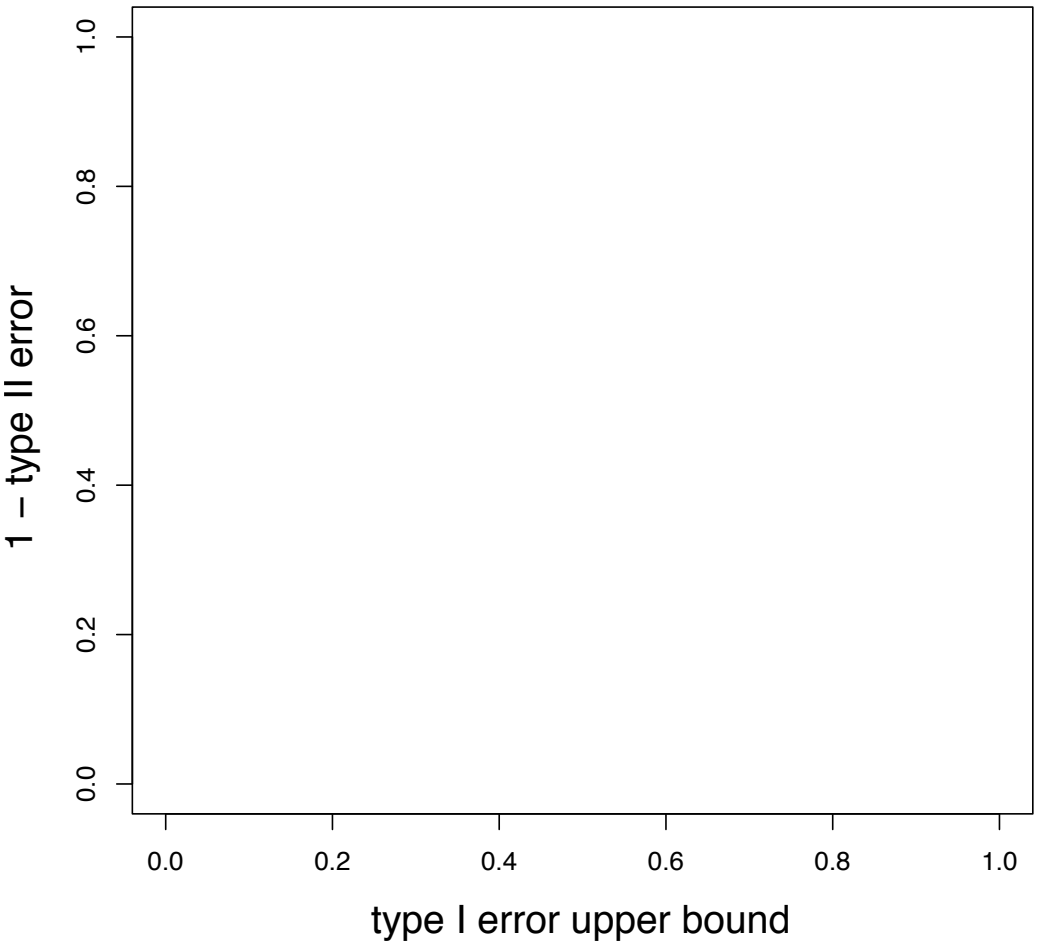
Population type I error controlled? YES

Choosing classifiers with population type I error control?



The empirical ROC space provides NO direct information on the population type I error control.

Choosing classifiers with population type I error control?



NP-ROC

$\Leftarrow$ NP classification methods

NP-ROC Band

Question: now, we have a high-probability type I error control, how about type II error? For this, we would need a left-out sample for class 1

Revised sample splitting:

- (1) mixed classed 0 and 1 sample $\overset{\text{algorithm}}{\Longrightarrow}$ trained model
- (2) left-out class 0 sample $\overset{\text{model}}{\Longrightarrow}$ classification scores
- (3) left-out class 1 sample $\overset{\text{evaluation}}{\Longrightarrow}$ type II error lower and upper bounds

Remark: sometimes we need to pay a price to know how well we will do in the future

Illustration of the band construction process

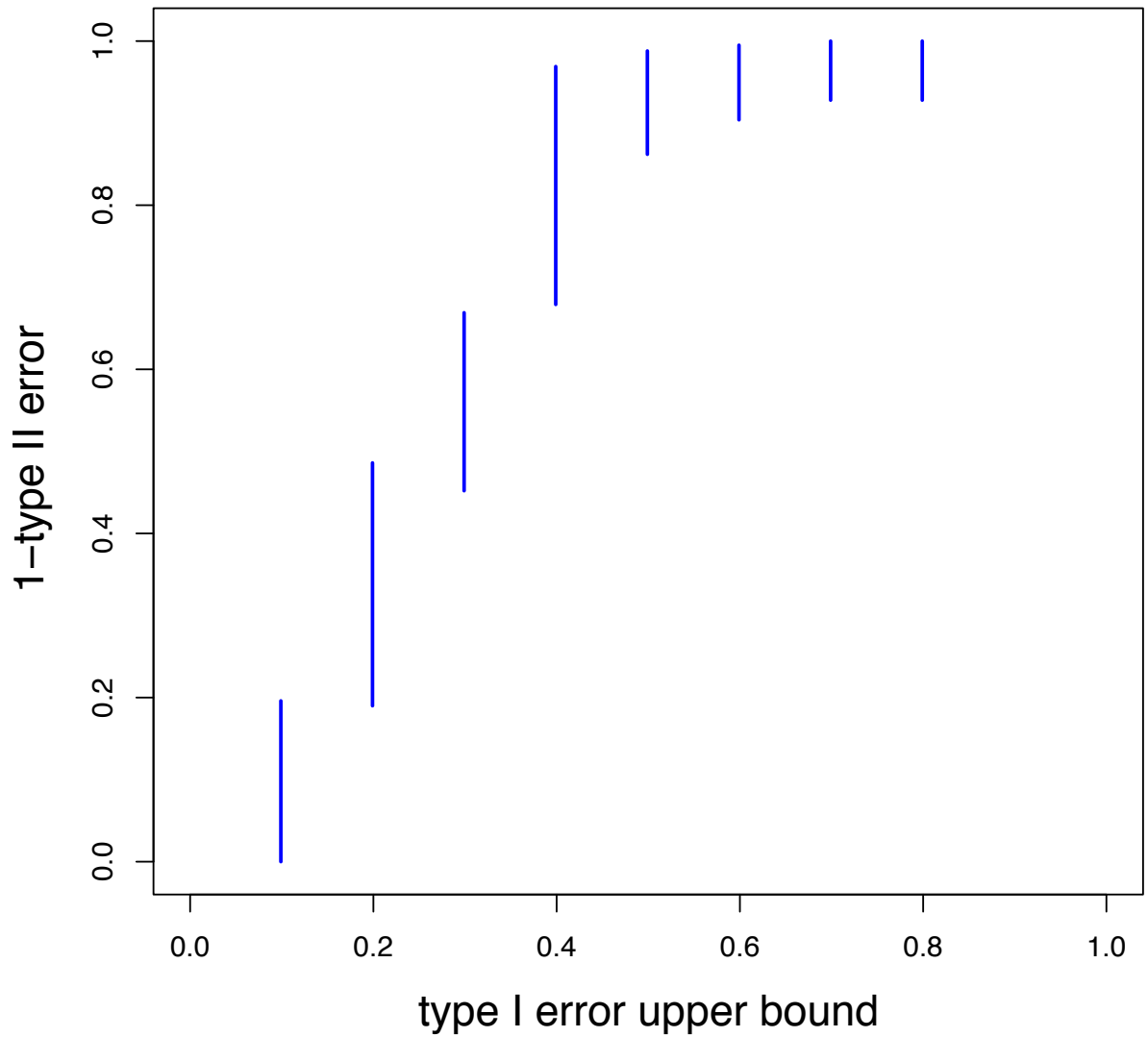
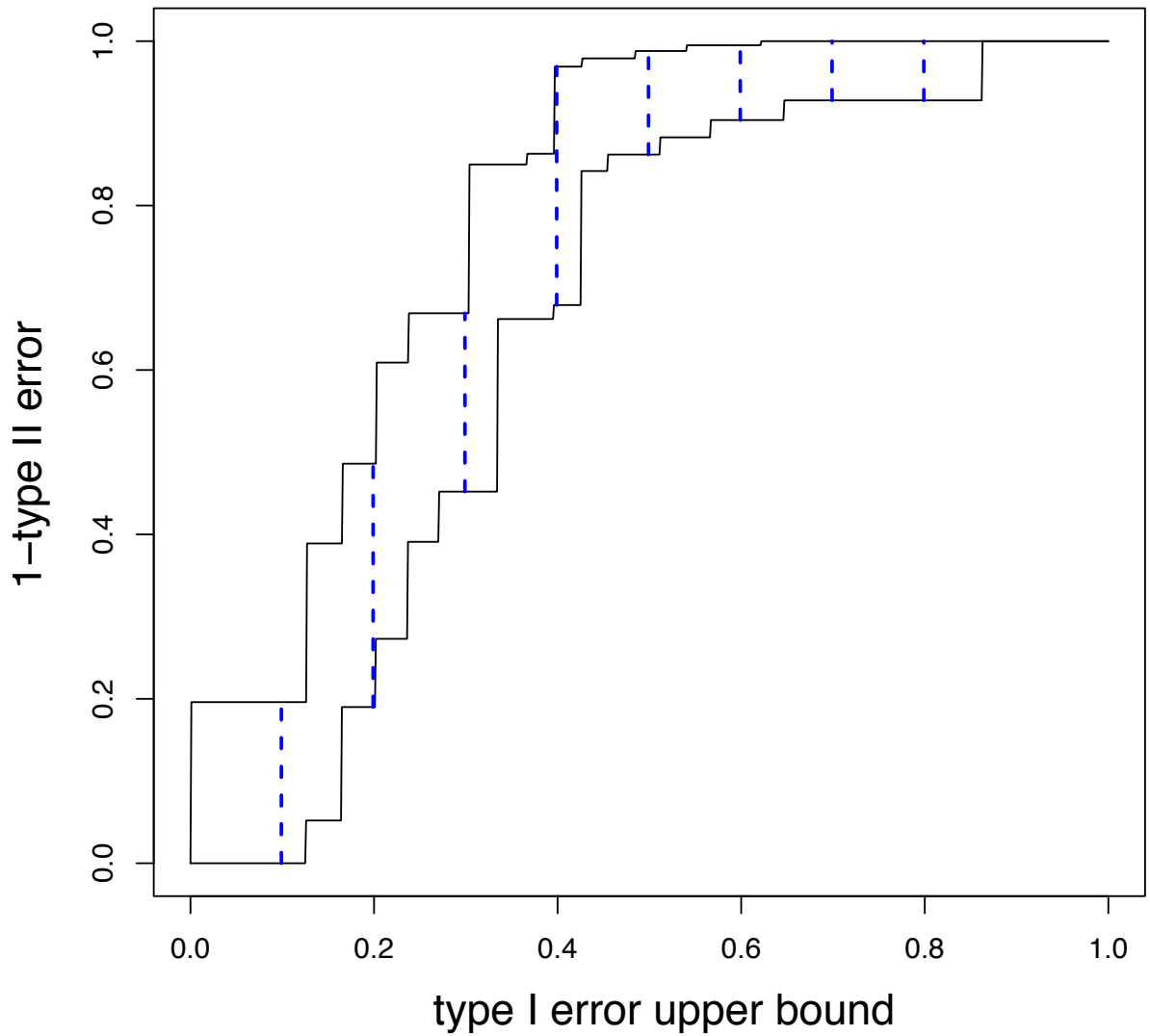
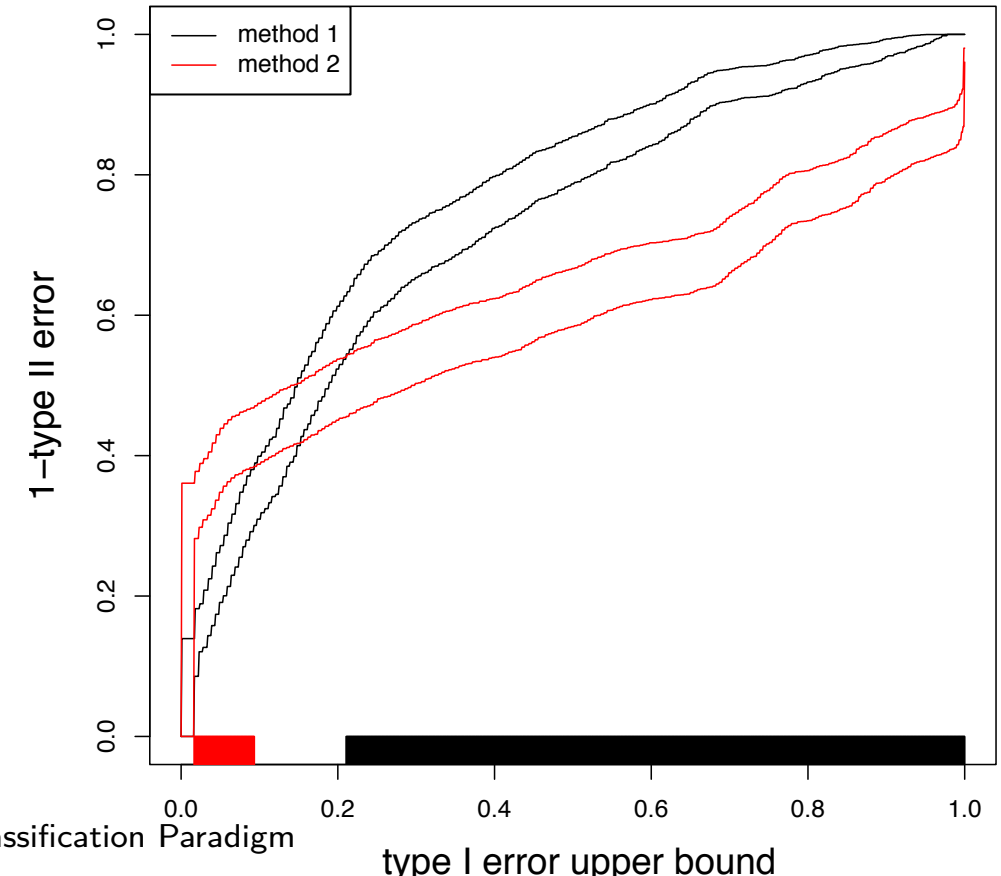


Illustration of the band construction process



Comparison of two NP-ROC bands

$(X_1|Y=0) \sim \mathcal{N}(0,1)$, $(X_1|Y=1) \sim \mathcal{N}(1,1)$, $(X_2|Y=0) \sim \mathcal{N}(0,1)$ and $(X_2|Y=1) \sim \mathcal{N}(1,6)$ with $\mathbb{P}(Y=0) = \mathbb{P}(Y=1) = 0.5$.
$n = 1,000$, $\delta = 0.1$.
We would like to investigate the Linear Discriminant Analysis that uses only X_1 (referred to as f_1) or only X_2 (referred to as f_2)



Ongoing work: feature ranking under the NP paradigm

Motivation

In automated disease diagnosis using gene expression data

- Which genes or gene sets are of the highest diagnostic power?
- Do they also play key roles in disease development and progression?

Misdiagnosing a cancer patient as healthy is much more severe than misdiagnosing a healthy patient with cancer!

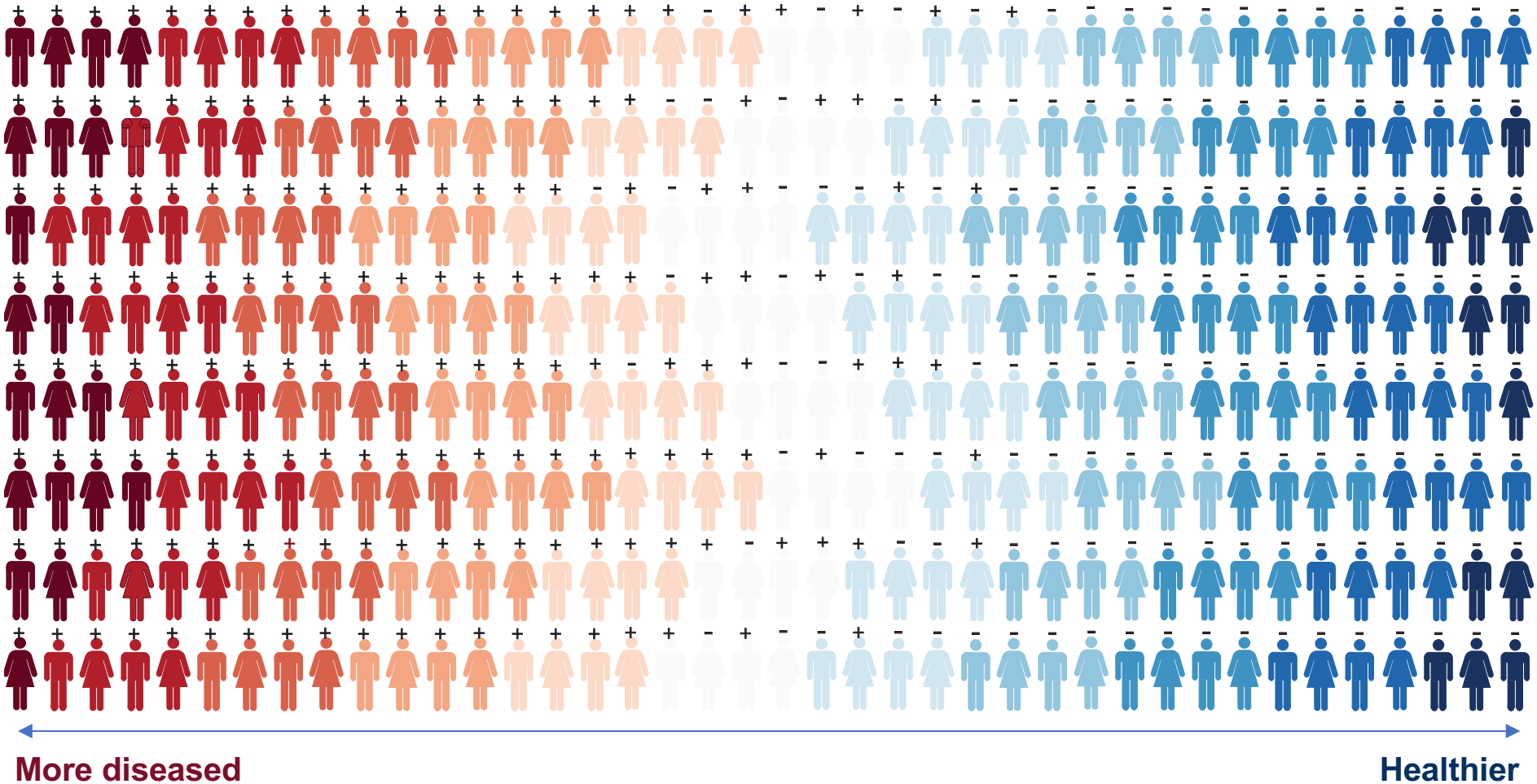
- Gene ranks obtained by minimizing the overall error rate is NOT a proper goal
- A more reasonable approach:
  rank genes by the less severe error rate while controlling the more severe error rate under some user-defined threshold α, usually a small value such as 5%

Summary

- Binary classification
  - Key question: where is the randomness?
- NP classification
  - Control of type I error with high probability
  - NP umbrella algorithm
- NP-ROC
  - NP-ROC bands can be used to compare two classifiers
  - Help choose α adaptively

Controlling the population error is important

The population

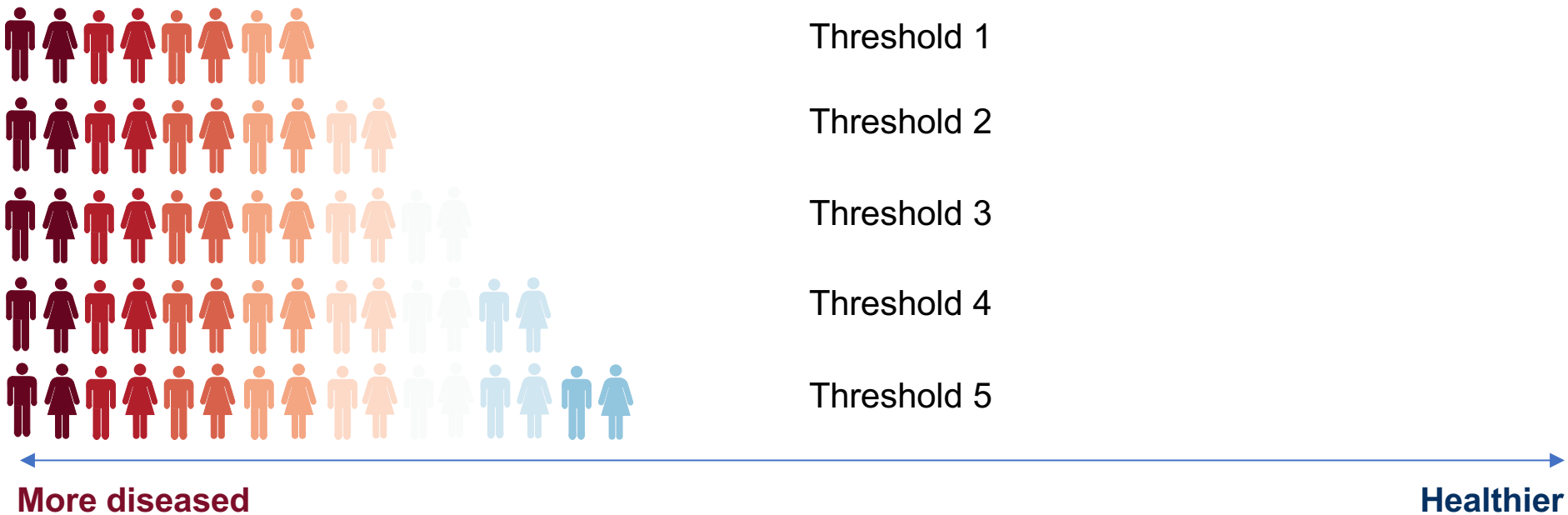


https://youtu.be/vbeeHqJ_PHY

Controlling the population error is important

Where to set the threshold?

Question:
If doctors would like to control the false negative rate under 1% while minimizing the false positive rate, what should be the diagnosis threshold?



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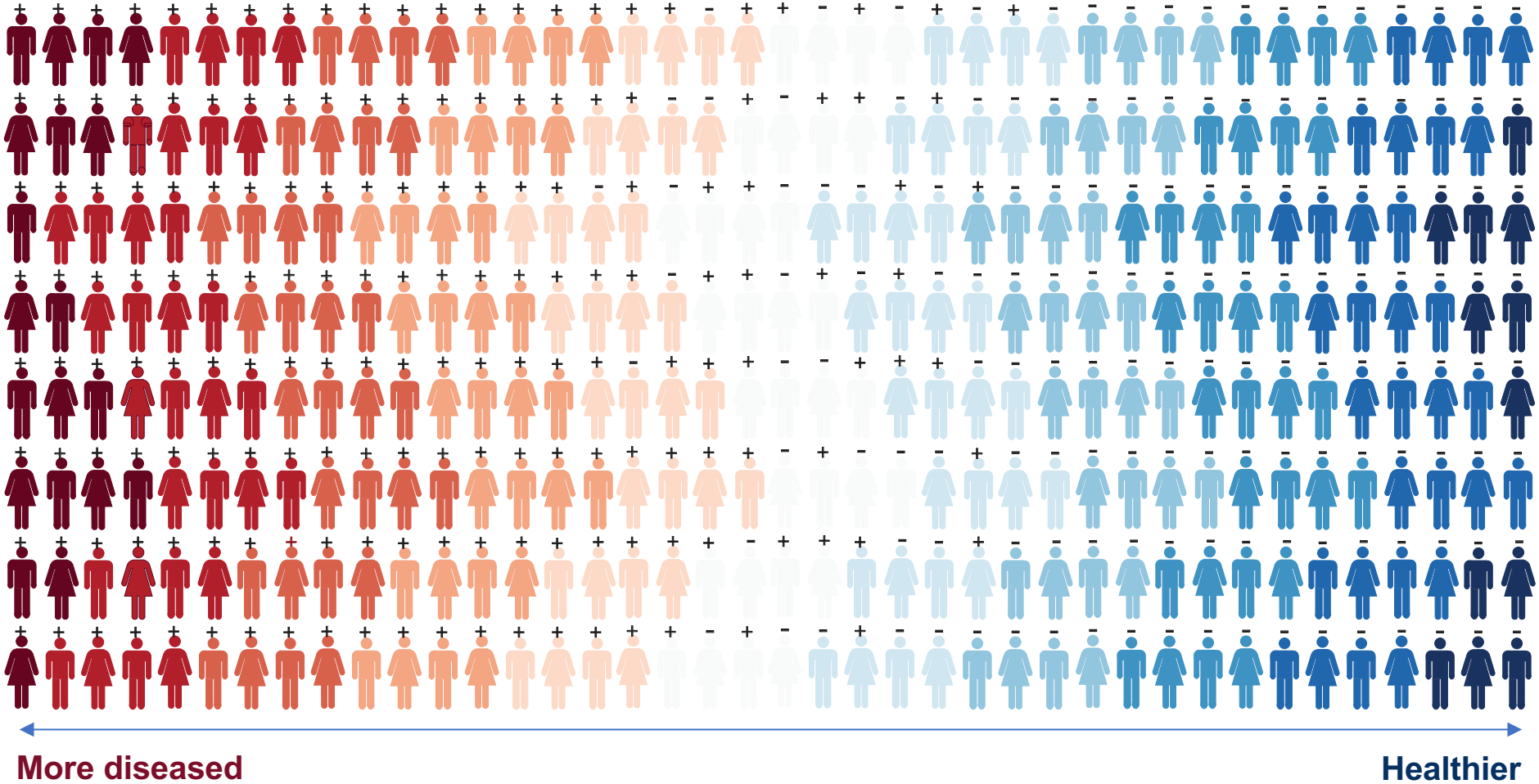
Controlling the population error is important

Setting the threshold is not difficult when observing the population



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Controlling the population error is important

Setting the threshold is not difficult when observing the population

Threshold 1

Threshold 2

Threshold 3

Threshold 4 ⭐

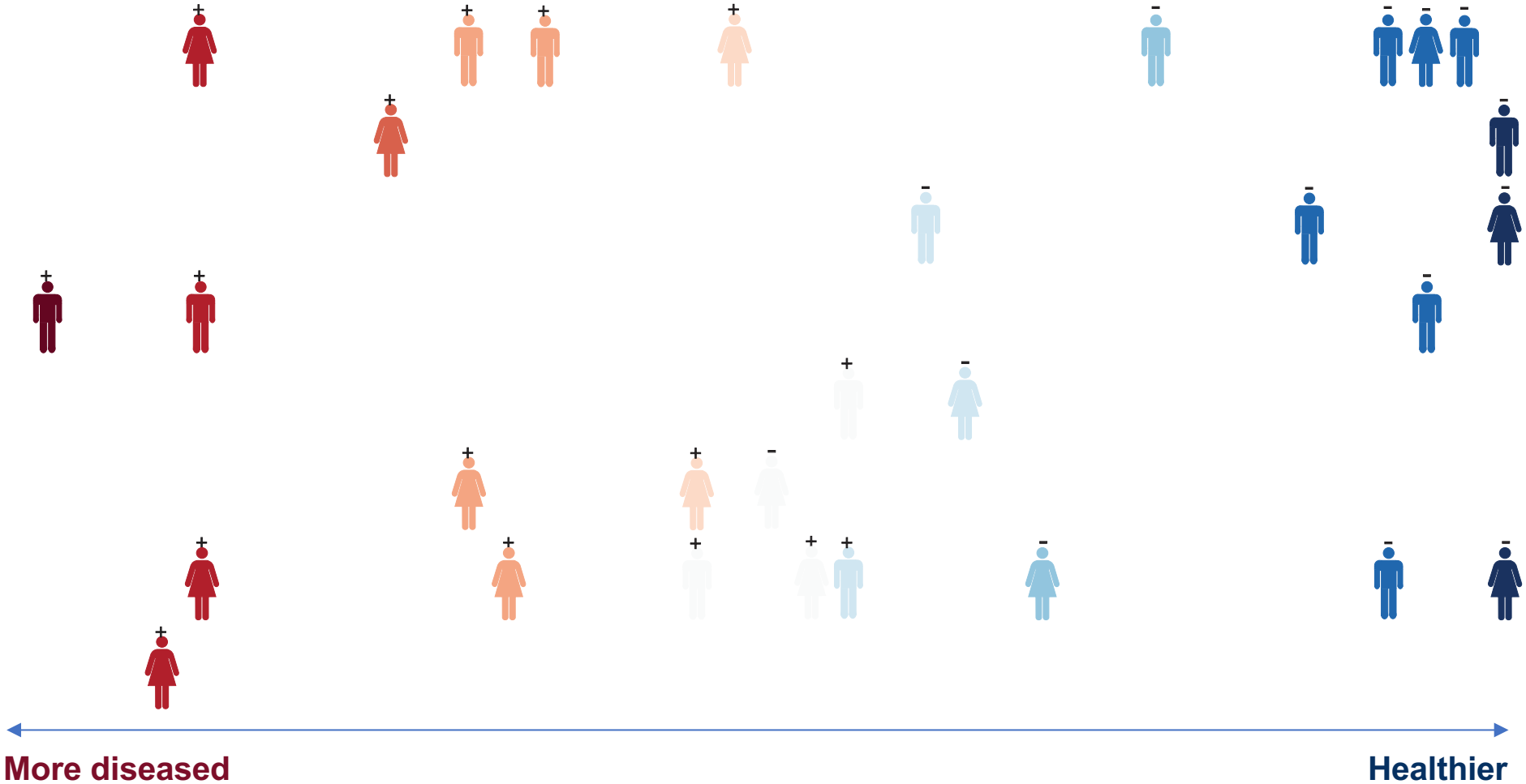
Threshold 5

More diseased — **Healthier**

https://youtu.be/vbeeHqJ_PHY

Controlling the population error is important

However in reality, we only observe a random sample from the population



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Controlling the population error is important

Problem arises if we set the threshold such that the false negative rate (FNR) on a random sample equals 1%

Threshold 1

Threshold 2 ⟶ FNR on the population = 7% 😭

Threshold 3

Threshold 4

Threshold 5

More diseased — **Healthier**

https://youtu.be/vbeeHqJ_PHY

Controlling the population error is important

As we observe more and more random samples...

How likely will we choose each threshold?

Threshold 1 (5%)

Threshold 2 (15%)

Threshold 3 (30%)

Threshold 4 ⭐ (35%)

Threshold 5 (15%)

About half the chance we will choose a threshold with FNR on the population greater than 1% 😭

More diseased ◄——————————————————► **Healthier**

https://youtu.be/vbeeHqJ_PHY

Paper and Software

SCIENCE ADVANCES | RESEARCH ARTICLE

RESEARCH METHODS

Neyman-Pearson classification algorithms and NP receiver operating characteristics

Xin Tong,[1*†] Yang Feng,[2†] Jingyi Jessica Li[3*]

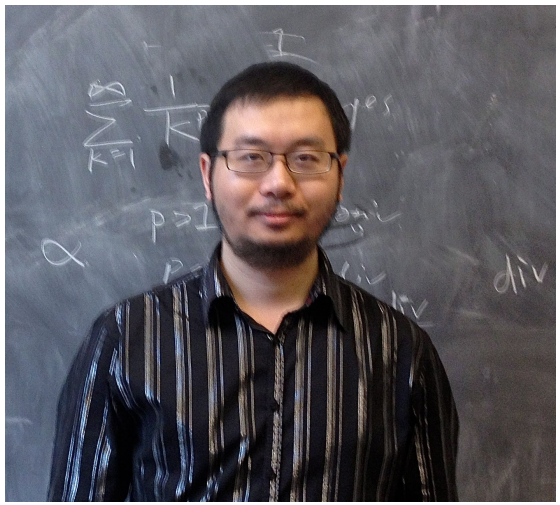
In many binary classification applications, such as disease diagnosis and spam detection, practitioners commonly face the need to limit type I error (that is, the conditional probability of misclassifying a class 0 observation as class 1) so that it remains below a desired threshold. To address this need, the Neyman-Pearson (NP) classification paradigm is a natural choice; it minimizes type II error (that is, the conditional probability of misclassifying a class 1 observation as class 0) while enforcing an upper bound, α, on the type I error. Despite its century-long history in hypothesis testing, the NP paradigm has not been well recognized and implemented in classification schemes. Common practices that directly limit the empirical type I error to no more than α do not satisfy the type I error control objective because the resulting classifiers are likely to have type I errors much larger than α, and the NP paradigm has not been properly implemented in practice. We develop the first umbrella algorithm that implements the NP paradigm for all scoring-type classification methods, such as logistic regression, support vector machines, and random forests. Powered by this algorithm, we propose a novel graphical tool for NP classification methods: NP receiver operating characteristic (NP-ROC) bands motivated by the popular ROC curves. NP-ROC bands will help choose α in a data-adaptive way and compare different NP classifiers. We demonstrate the use and properties of the NP umbrella algorithm and NP-ROC bands, available in the R package nproc, through simulation and real data studies.

R package `nproc`

https://CRAN.R-project.org/package=nproc

Email: jli@stat.ucla.edu

Acknowledgements



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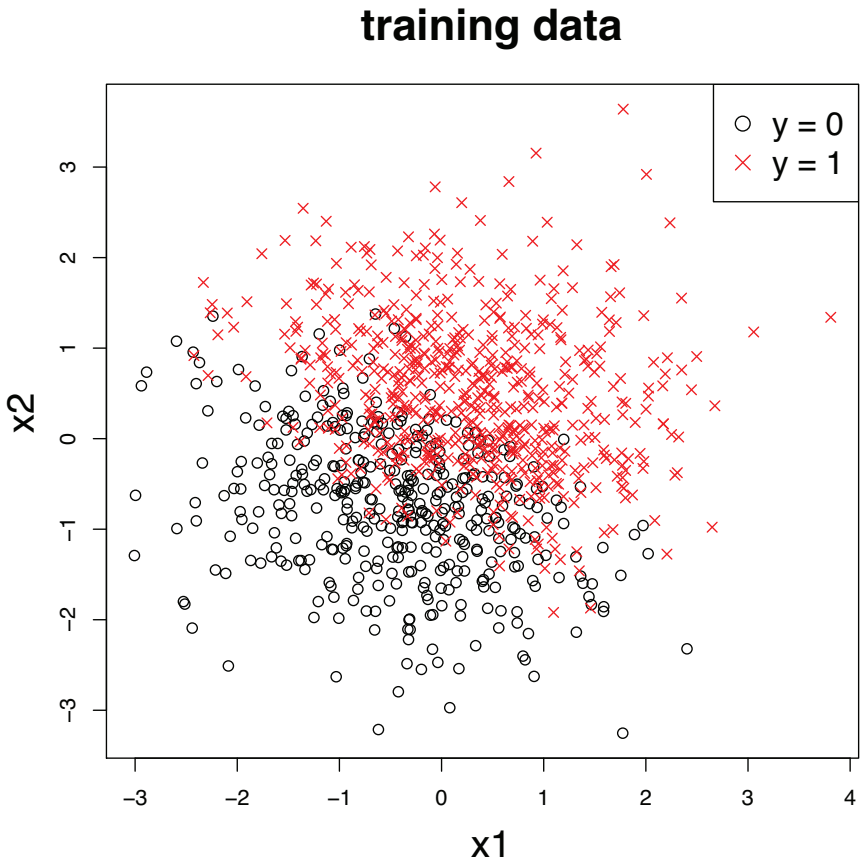
(Columbia)

Yiling Chen
(UCLA)

R package `nproc` and simulation examples

- Package nproc on CRAN:
  ```
  > library(nproc)
  ```
- Toy data dat simulated from a logistic model
  $\mathbb{P}(Y = 1) = 1/\left(1 + \exp\{-(1 + 2X_1 + 3X_2)\}\right)$, X_1, $X_2 \sim N(0, 1)$.



Logistic regression

- We first train a logistic regression model on the training data under the classical paradigm.

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> lr_model1 <- glm(y~x1+x2, data=dat, family="binomial")
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```
> summary(lr_model1_err)
Min.     1st Qu.   Median   Mean     3rd Qu.   Max.
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- We next train a logistic regression model on the training data under the NP paradigm with type I error bound $\alpha = 0.05$.

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> lr_model2 <- npc(x=x,y=y,method='logistic',alpha=.05)
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```
> lr_model2 <- npc(x=x,y=y,method='logistic',alpha=.05)
```

- Then we also apply the trained model `lr_model2` to the test data.

```
> summary(lr_model2_err)
Min.       1st Qu.    Median     Mean       3rd Qu.    Max.
0.009732   0.027830   0.033960   0.034400   0.040880   0.065040
```