MS IA : MDI721
Statistical hypothesis testing for linear model

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Outline

General principle

Context

- We observe $X_1, \dots, X_n$ from a common distribution $\mathcal{P}$
- We are interested in $\theta \in \Theta$, a parameter of $\mathcal{P}$

Goal

To decide whether an assumption on θ is likely (or not)

$$\mathcal{H}_0 = \{\theta \in \Theta_0\}$$

against some alternative

$$\mathcal{H}_1 = \{\theta \in \Theta_1\}$$

Call $\mathcal{H}_0$ the null hypothesis, $\mathcal{H}_1$: the alternative

General principle

Means

Determine a test statistic $T(X_1, \ldots, X_n)$ and a region R such that if

$$T(X_1, \ldots, X_n) \in R \;\Rightarrow\; \text{we reject } \mathcal{H}_0$$

In other words the observed data discriminates between H_0 and H_1

Hypothesis testing for “heads or tails”

When flipping a coin the model is a Bernoulli distribution with parameter p, $\mathcal{B}(p)$.

Is the coin fair?

$$\mathcal{H}_0 = \{p = 0.5\} \quad \text{against} \quad \mathcal{H}_1 = \{p \neq 0.5\}$$

Is the coin possibly unfair?

$$\mathcal{H}_0 = \{0.45 \leq p \leq 0.55\} \quad \text{against} \quad \mathcal{H}_1 = \{p \notin [0.45, 0.55]\}$$

Do we reject or do we accept ?

In most practical situations, $\mathcal{H}_0$ is simple, i.e.,

$$\Theta_0 = \{\theta_0\}$$

and $\Theta_1 = \Theta \backslash \Theta_0$ is large

($\mathcal{H}_0$ is often an hypothesis on which we care particularly, e.g., something acknowledged to be true, easy to formulate)

We only reject $\mathcal{H}_0$

If $\mathcal{H}_0$ is not rejected we cannot conclude $\mathcal{H}_0$ is true because $\mathcal{H}_1$ is too general

e.g. $\{p \in [0, 0.5[\cup]0.5, 1]\}$ can not be rejected!

2 types of error

	$\mathcal{H}_0$	$\mathcal{H}_1$
$\mathcal{H}_0$ is not rejected	Correct	Wrong (False negative)
$\mathcal{H}_0$ is rejected	Wrong (False positive)	Correct

- Type I: probability of a wrong reject

$$\mathbb{P}(T(X_1, \ldots, X_n) \in R \mid \mathcal{H}_0)$$

- Type II: probability of wrong non-reject

$$\mathbb{P}(T(X_1, \ldots, X_n) \notin R \mid \mathcal{H}_1)$$

Significance level and power

Significance level α if

$$\limsup_{n\to+\infty} \mathbb{P}(T(X_1,\ldots,X_n) \in R \mid \mathcal{H}_0) \leq \alpha$$

(We speak of 95%-test when α is 0.05%)

Consistency

A test statistics (given by $T(X_1,\ldots,X_n)$ and a region R) is said to be α-consistent if the significant level is α and if the power goes to one, i.e.,

$$\limsup_{n\to+\infty} \mathbb{P}(T(X_1,\ldots,X_n) \in R \mid \mathcal{H}_0) \leq \alpha$$

$$\lim_{n\to\infty} \mathbb{P}(T(X_1,\ldots,X_n) \in R \mid \mathcal{H}_1) = 1$$

Test statistic and reject region

Goal: to build a α-consistent test

(1) Define the test statistic $T(X_1, \ldots, X_n)$ and the level α you wish

(2) Do some maths to determine a reject region R that achieves a significance level α

(3) Prove the consistency

(4) Rule decision: reject whenever $\boxed{T_n(X_1, \ldots, X_n) \in R}$

Famous tests

- Test of the equality of the mean for 1 sample
- Test of the equality of the means between 2 samples
- Chi-square test for the variance
- Chi-square test of independence
- Regression coefficient non-effects test

Example: Gaussian mean

- Model: $\Theta = \mathbb{R}$, $\mathbb{P}_\theta = \mathcal{N}(\theta, 1)$
- Observe $(X_1, \ldots, X_n)$ i.i.d. from this model
- Null hypothesis: $\mathcal{H}_0 : \{\theta = 0\}$
- Under $\mathcal{H}_0$, $\quad T_n(X_1, \ldots, X_n) = \frac{1}{\sqrt{n}} \sum_i X_i \sim \mathcal{N}(0, 1)$
- Critical region for T_n ? Gaussian quantile:

$$\mathbb{P}(T_n \in [-1.96, 1.96] \mid \mathcal{H}_0) = 0.95$$

- Take $R =]-\infty, -1.96[\cup]1.96, +\infty[$.
- **Numerical example**: If $T_n = 1.5$, we do **not** reject $\mathcal{H}_0$ at level 95%

Usage of the p-value

- The decision to accept or reject $\mathcal{H}_0$ is subject to the chosen significance level α.
- To avoid making this choice in advance, in particular in software, the notion of the p-value is used to represent the result of a test.
- **The p-value is the probability that, under $\mathcal{H}_0$, the test statistic T_n takes a value at least as extreme as its observed value.**
- Relation to the critical region:
    - If the test is one-sided with $R = \{t \,|\, t > c\}$ then for the observed T_n the p-value is $\mathbb{P}(T > t_0 \,|\, \mathcal{H}_0)$.
    - If the test is one-sided with $R = \{t \,|\, t < c\}$ then for the observed T_n the p-value is $\mathbb{P}(T < T_n \,|\, \mathcal{H}_0)$.
    - If the test is two-sided with $R = \{t \,|\, t \in] -\infty; c_1) \cup (c_2; +\infty[\}$ then for the observed T_n the p-value is $2\mathbb{P}(T < T_n \,|\, H_0)$ if T_n is smaller than the median, and $2\mathbb{P}(T > T_n \,|\, H_0)$ if T_n is larger than the median.

Usage of the p-value: example

- Model: $\Theta = \mathbb{R}$, $\mathbb{P}_\theta = \mathcal{N}(\theta, 1)$
- Observe $(X_1, \ldots, X_n)$ i.i.d. from this model
- Null hypothesis: $\mathcal{H}_0 : \{\theta \leq 5\}$
- Under $\mathcal{H}_0$, $\quad T_n(X_1, \ldots, X_n) = \frac{\overline{X}_n - 5}{\frac{1}{\sqrt{n}}} \sim \mathcal{N}(0, 1)$

The test decision:

- Reject $\mathcal{H}_0$ if $\overline{X}_n > 5 + z_{1-\alpha}\frac{1}{\sqrt{n}}$.

Using the p-value:

- Assume $n = 10$ and $\overline{X}_n = 5.75$.
- The p-value equals $\mathbb{P}(\overline{X} > 5.75)$ with $\overline{X} \sim \mathcal{N}(5, \frac{1}{10})$, *i.e.* $\mathbb{P}(Z > 2.3717)$ with $Z \sim \mathcal{N}(0, 1)$, which equals 0.0089.
- This indicates directly that one should reject at a level 0.05 and even 0.01.
- If the test would be two sided, *i.e.* with $\mathcal{H}_0 : \{\theta = 5\}$, the p-value for $\overline{X}_n = 5.75$ would be $0.0089 \times 2 = 0.0178$ implying **reject** at a level 0.05 but **not** 0.01.

Test of no-effect : Gaussian case

Gaussian Model

$$y_i = \theta_0^\star + \sum_{k=1}^{p} \theta_k^\star x_{i,k} + \varepsilon_i$$

$$x_i^\top = (1, x_{i,1}, \dots, x_{i,p}) \in \mathbb{R}^{p+1} \text{ (deterministic)}$$

$$\varepsilon_i \overset{i.i.d}{\sim} \mathcal{N}(0, \sigma^2), \text{ for } i = 1, \dots, n$$

Theorem

Let $X = (x_1, \dots, x_n)^\top \in \mathbb{R}^{n \times (p+1)}$ of full rank, and $\widehat{\sigma}^2 = \|\mathbf{y} - X\widehat{\boldsymbol{\theta}}\|_2^2/(n-(p+1))$, then

$$\widehat{T}_j = \frac{\widehat{\theta}_j - \theta_j^*}{\widehat{\sigma}\sqrt{(X^\top X)_{j,j}^{-1}}} \sim \mathcal{T}_{n-(p+1)}$$

where $\mathcal{T}_{n-p}$ is a Student law (with $n-(p+1)$ degrees of freedom)

Test of no-effect : Gaussian case

Null hypothesis

Aim is to test

$$\mathcal{H}_0 : \theta_j^* = 0$$

equivalently, $\Theta_0 = \{\theta \in \mathbb{R}^p : \theta_j = 0\}$

Under $\mathcal{H}_0$, we know the value of $\widehat{T}_j$:

$$T_j := \frac{\widehat{\theta}_j}{\widehat{\sigma}\sqrt{(X^\top X)^{-1}_{j,j}}} \sim \mathcal{T}_{n-(p+1)}$$

Choosing $R = [-t_{1-\alpha/2}, t_{1-\alpha/2}]^c$ with $t_{1-\alpha/2}$ the $1-\alpha/2$-quantile of $\mathcal{T}_{n-(p+1)}$, we decide to reject $\mathcal{H}_0$ whenever

$$|\widehat{T}_j| > t_{1-\alpha/2}$$

Test of no-effect : Random-design case

Random design Model

$$y_i = \theta_0^\star + \sum_{k=1}^{p} \theta_k^\star \mathsf{x}_{i,k} + \varepsilon_i$$

$$\mathsf{x}_i^\top = (1, \mathsf{x}_{i,1}, \dots, \mathsf{x}_{i,p}) \in \mathbb{R}^{p+1}$$

$$(\varepsilon_i, \mathsf{x}_i) \overset{i.i.d}{\sim} (\varepsilon, \mathsf{x}), \text{ for } i = 1, \dots, n$$

$$\mathbb{E}(\varepsilon|\mathsf{x}) = 0, \ \mathbb{V}\mathrm{ar}(\epsilon|\mathsf{x}) = \sigma^2$$

Theorem

If $\mathrm{var}(\mathsf{x})$ has full rank, then

$$\widehat{T}_j = \frac{\widehat{\theta}_j - \theta_j^*}{\widehat{\sigma}\sqrt{(X^\top X)^{-1}_{j,j}}} \xrightarrow{\mathrm{d}} \mathcal{N}(0,1)$$

Test of no-effect : Random-design case

Null hypothesis

Aim is to test

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Under $\mathcal{H}_0$, we know the value of $\widehat{T}_j$:

$$T_j := \frac{\widehat{\theta}_j}{\widehat{\sigma}\sqrt{(X^\top X)^{-1}_{j,j}}} \xrightarrow{\mathrm{d}} \mathcal{N}(0,1)$$

Choosing $R = [-z_{1-\alpha/2}, z_{1-\alpha/2}]^c$ with $z_{1-\alpha/2}$ the $1-\alpha/2$-quantile of $\mathcal{N}(0,1)$), we decide to reject $\mathcal{H}_0$ whenever

$$|\widehat{T}_j| > z_{1-\alpha/2}$$

Link between IC and test

Reminder (Gaussian model):

$$IC_\alpha := \left[\widehat{\theta}_j - t_{1-\alpha/2}\widehat{\sigma}\sqrt{(X^\top X)^{-1}_{j,j}}, \widehat{\theta}_j + t_{1-\alpha/2}\widehat{\sigma}\sqrt{(X^\top X)^{-1}_{j,j}}\right]$$

is a CI at level α for θ^*_j. Stating "$0 \in IC_\alpha$" means

$$|\widehat{\theta}_j| \leq t_{1-\alpha/2}\widehat{\sigma}\sqrt{(X^\top X)^{-1}_{j,j}} \quad \Leftrightarrow \quad \frac{|\widehat{\theta}_j|}{\widehat{\sigma}\sqrt{(X^\top X)^{-1}_{j,j}}} \leq t_{1-\alpha/2}$$

It is equivalent to accepting the hypothesis $\theta^*_j = 0$ at level α. The smallest α such that $0 \in IC_\alpha$ is called the ***p*-value**.

Rem: Taking α close to zero IC_α covers the full space, hence one can find (by continuity) an α achieving equality in the aforementioned equations.

Outline

“Diabetes” data set

patient	age x1	sex x2	bmi x3	bp x4	Serum measurements x5	x6	x7	x8	x9	x10	Resp y
1	59	2	32.1	101	157	93	38	4	4.9	87	151
2	48	1	21.6	87	183	103	70	3	3.9	69	75
...	...										...
...	...										...
441	36	1	30.0	95	201	125	42	5	5.1	85	220
442	36	1	19.6	71	250	133	97	3	4.6	92	57

$n = 442$ patients having diabetes, $p = 10$ variables “baseline” body mass index (bmi), average blood pressure (bp), *etc.*...have been measured.
Goal: predict disease progression one year in advance after the “baseline” measurement [EHJT04].

- Each variable of the data set from *sklearn* has been previously standardized.
- We apply an “expensive” version of the **forward variable selection** method (see, *e.g.*, [Zha09])

“Diabetes” data set

- We define a vector of covariates with intercept $\tilde{X} = (\mathbb{1}, \mathbf{x}_1, \ldots, \mathbf{x}_{10})$.

Step 0

- for each variable $\tilde{X}_k$, $k = 1, \ldots, 11$, we consider the model

$$\mathbf{y} \simeq \beta_k \mathbf{x}_k$$

- we test whether its regression coefficient equals zero, *i.e.*

$$H_0 : \beta_k = 0$$

  using the statistic $\frac{\widehat{\beta}_k}{\widehat{s}_k}$ with $\widehat{s}_k$ being the estimated standard deviation.

- we compare all of the p-values, and keep the one possessing the smallest p-value. We save the residuals in the vector $\mathbf{r}_0$.

“Diabetes” data set

Step ℓ

We have selected ℓ variable(s) : $\tilde{X}^{(\ell)} \in \mathbb{R}^{\ell}$. Those not selected are noted $\tilde{X}^{(-\ell)} \in \mathbb{R}^{p-\ell}$. We possess the vector of residuals $\mathbf{r}_{\ell-1}$ calculated on the previous step.

- for each variable $\mathbf{x}_k$ in $\tilde{X}^{(-\ell)}$, we consider the model

$$\mathbf{r}_{\ell-1} \simeq \beta_k \mathbf{x}_k$$

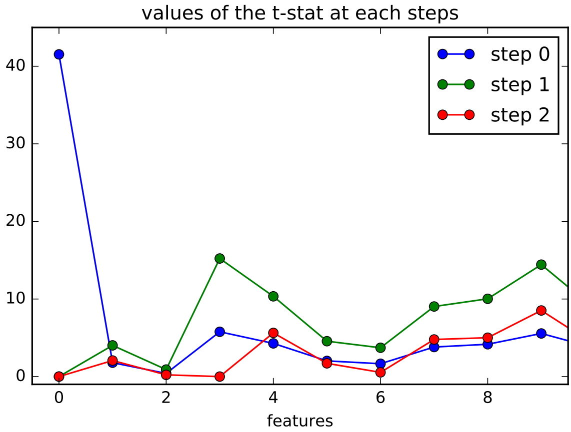
- we test if its regression coefficient equal zero, *i.e.*

$$H_0 : \beta_k = 0$$

  using the test statistic $\frac{\widehat{\beta}_k}{\widehat{s}_k}$ with $\widehat{s}_k$ being the estimated standard deviation.

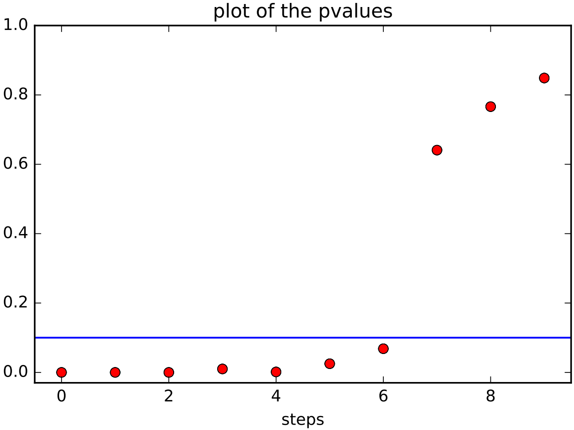
- we compare all of the p-values, and keep the one possessing the smallest p-value. We save the residuals in the vector $\mathbf{r}_\ell$.

Values of the test statistics at each step



- The test statistic of the selected variable is 0 on the following steps.
- The intercept is the first selected variable, then x_3, *etc...*

Values of the test statistics at each step



- Sequence of the selected variables wit the test size 0.1 :

[0, 3, ,9 ,5 ,4 ,2 ,7]

Outline

Medical context

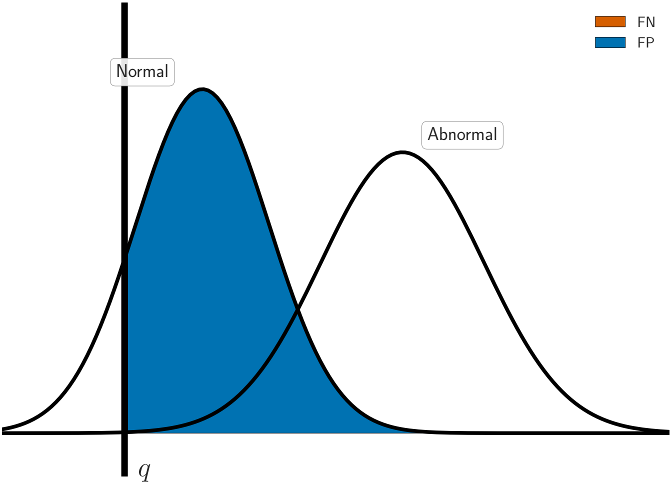
- A group of patients $i = 1, \ldots, n$ is followed for disease screening.
- For each individual, the test relies on a random variable $X_i \in \mathbb{R}$ and a threshold $q \in \mathbb{R}$

as soon as	$X_i > q$	the test is **positive**
o.w.		the test is **negative**

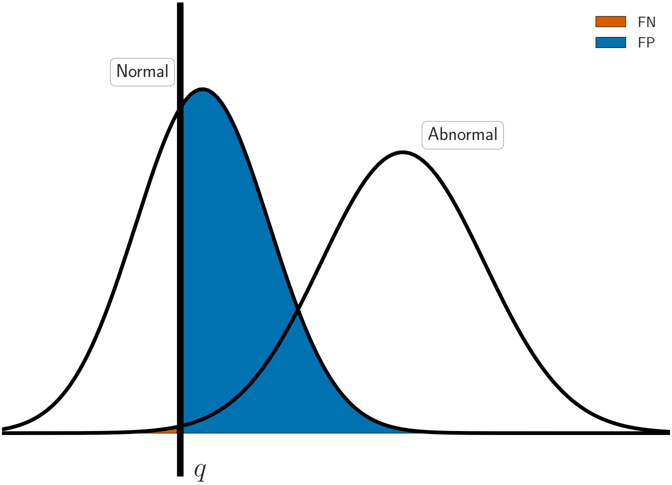
Set of possible configurations

	Normal H_0	Sick H_1
negative	true negative	false negative
positive	false positive	true positive

False positive vs. false negative



False positive vs. false negative



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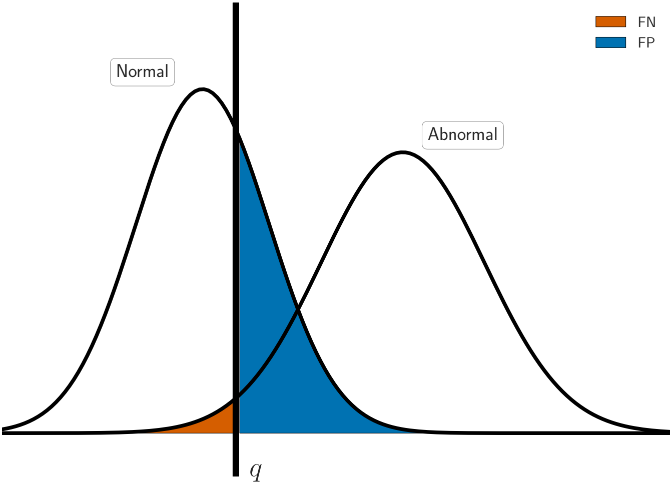

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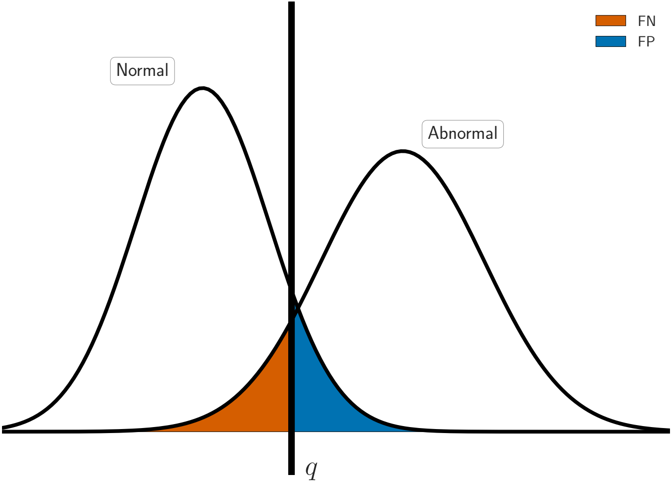

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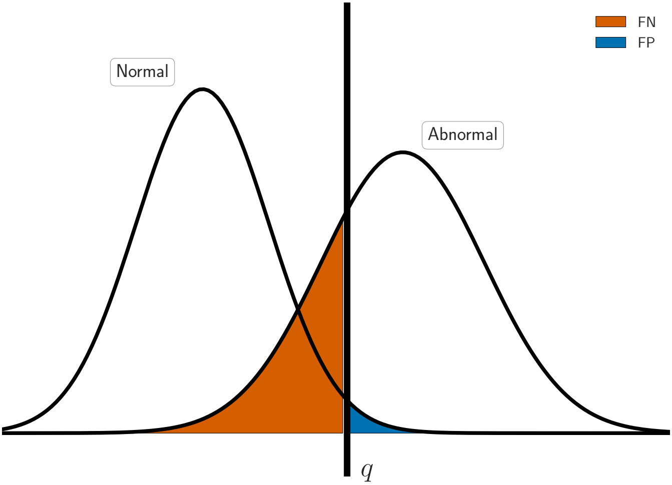

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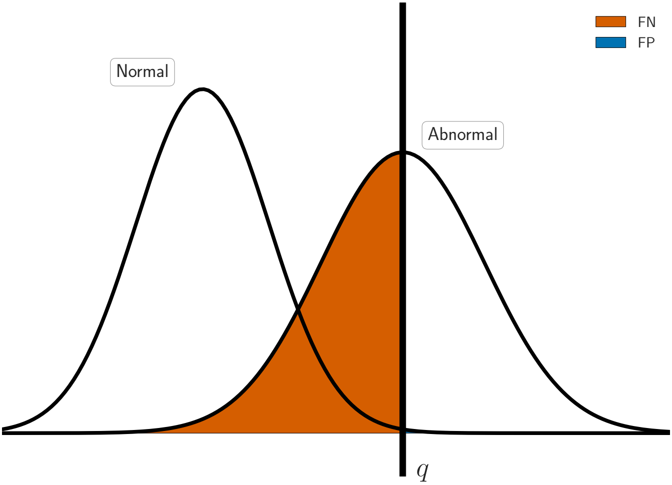

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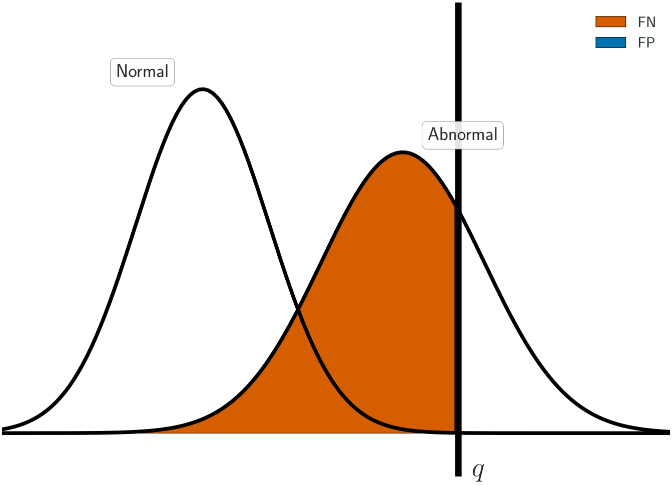

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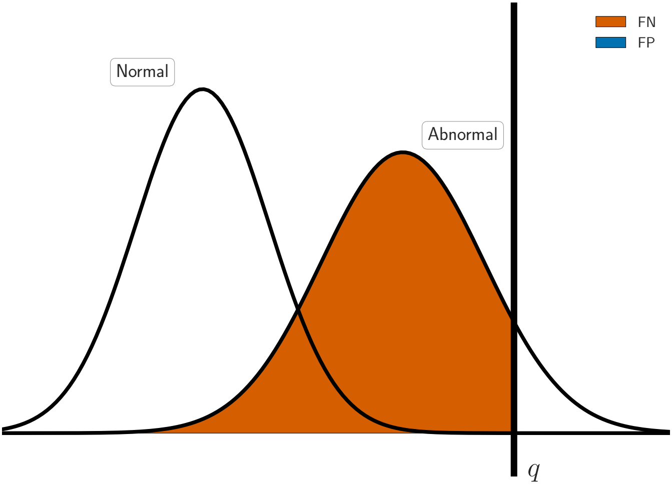

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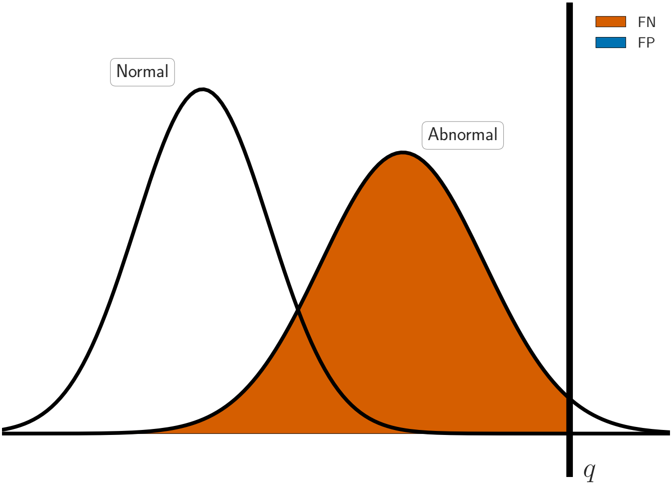


Sensitivity - Specificity

- Assumption: Normal individuals have the same c.d.f. F
- Assumption: Sick individual have the same c.d.f G

Definition

- Sensitivity : $\mathsf{Se}(q) = 1 - G(q)$ (1− type 2nd error)
- Specificity : $\mathsf{Sp}(q) = F(q)$ (1− type 1st error)

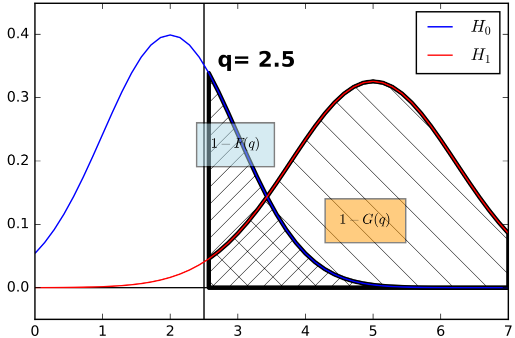
ROC curve

Definition

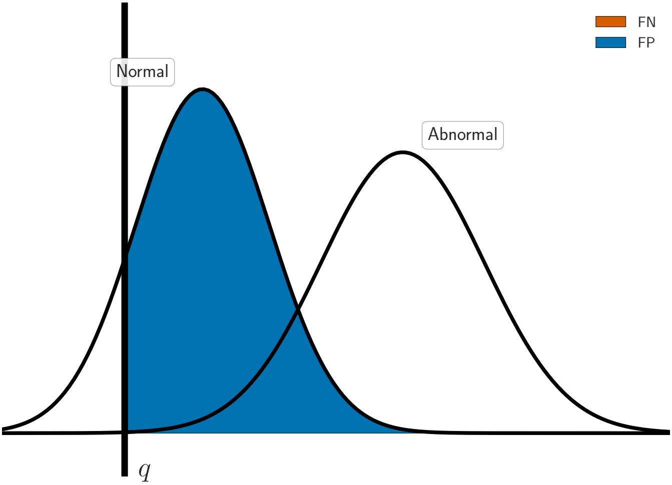
The ROC curve is the curve described by $(1 - \mathsf{Sp}(q), \mathsf{Se}(q))$, when $q \in \mathbb{R}$. Hence, it is the function $[0,1] \to [0,1]$

$$\mathsf{ROC}(t) = 1 - G(F^{-}(1-t))$$

where $F^{-}(1-t) = \inf\{x \in \mathbb{R} : F(x) \geq 1 - t\}$.



ROC Curve



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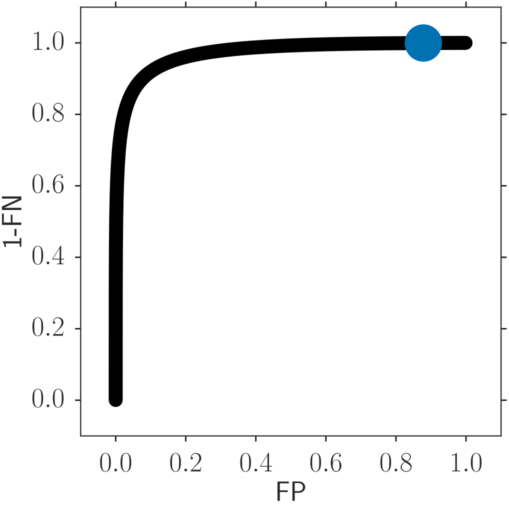

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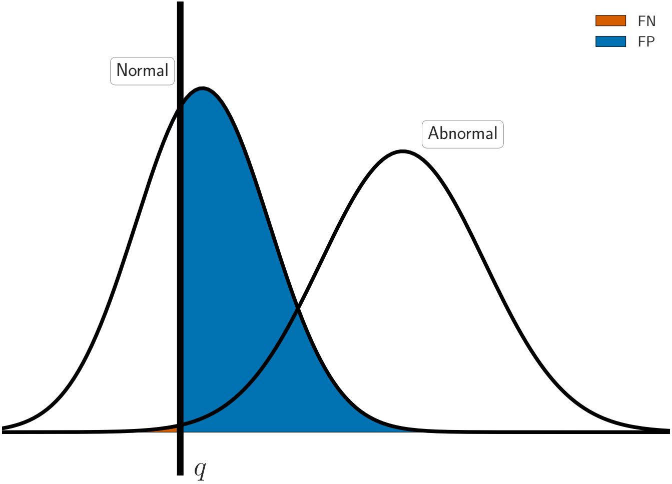

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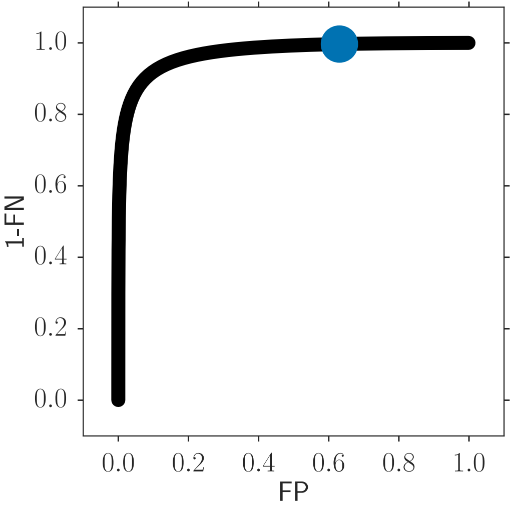

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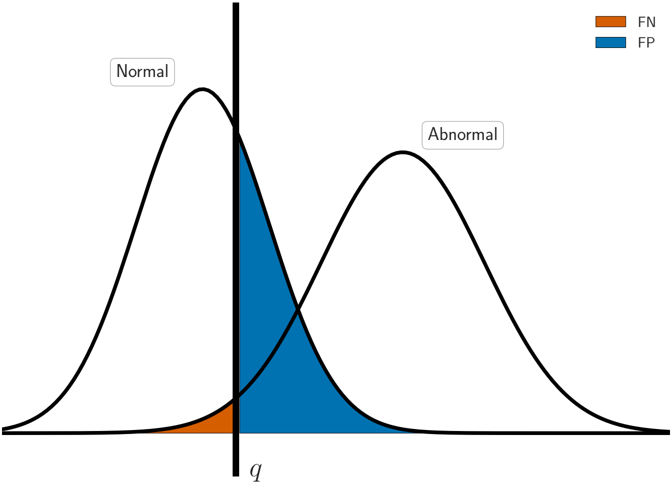

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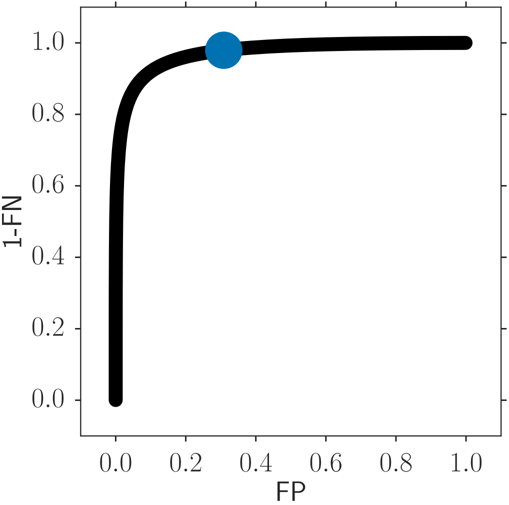

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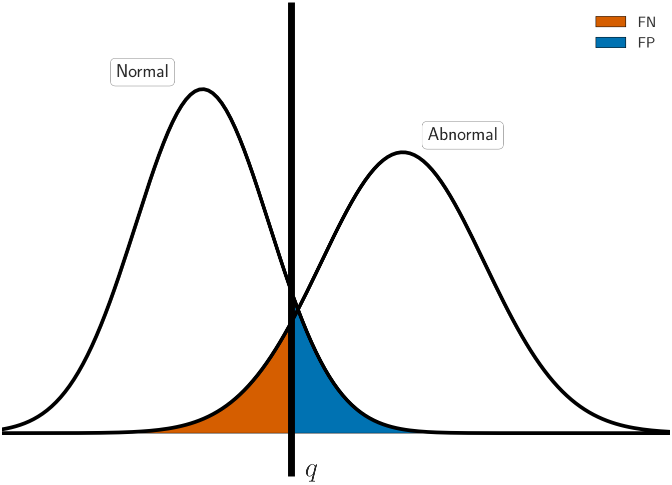

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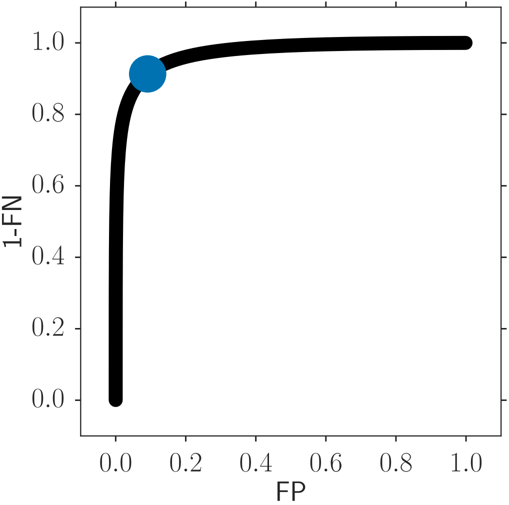

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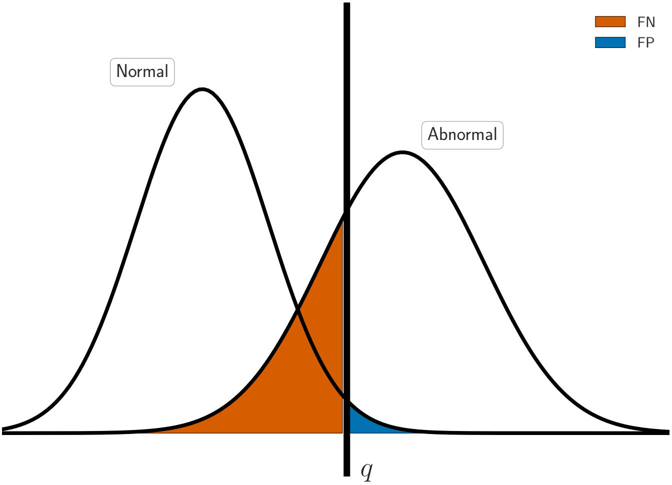

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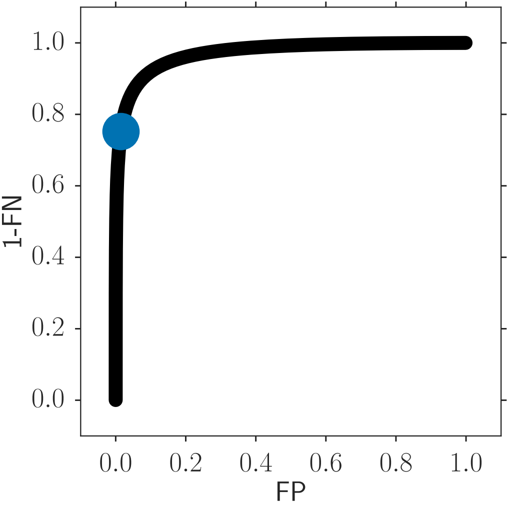

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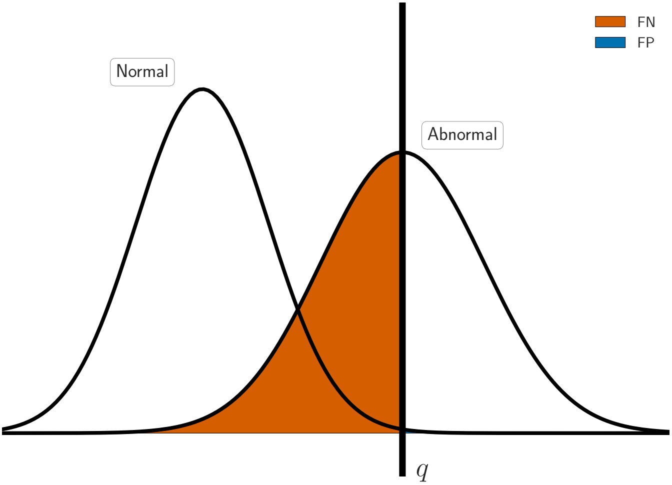

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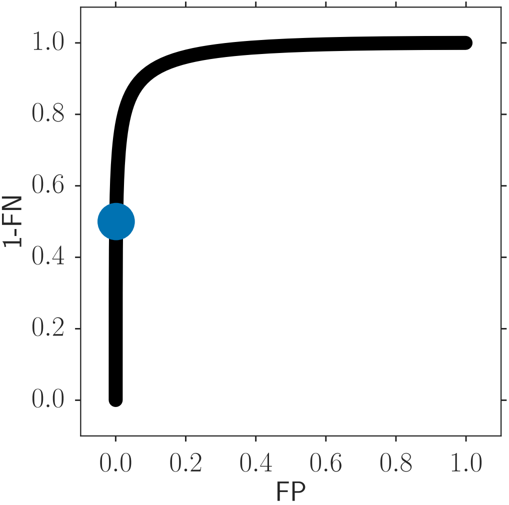

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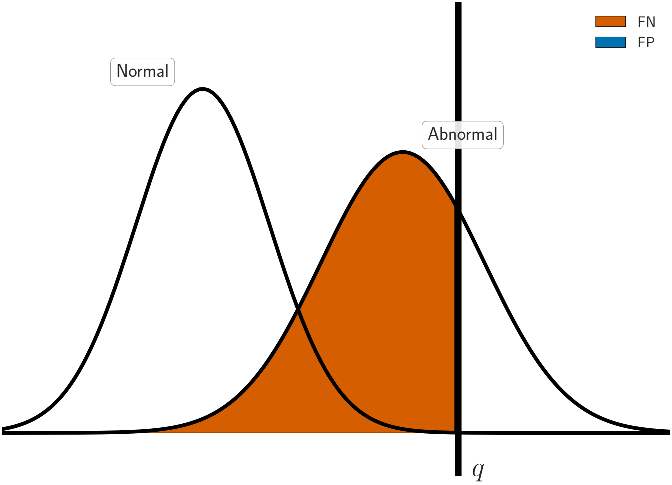

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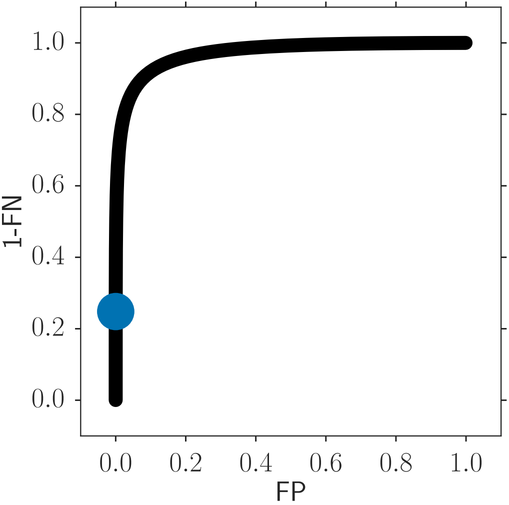

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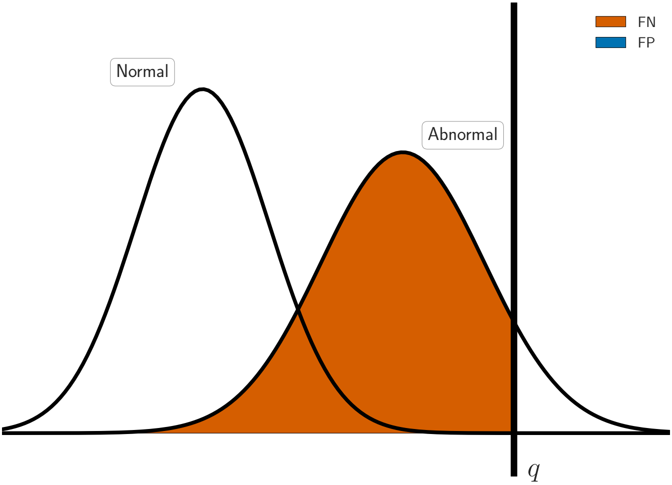

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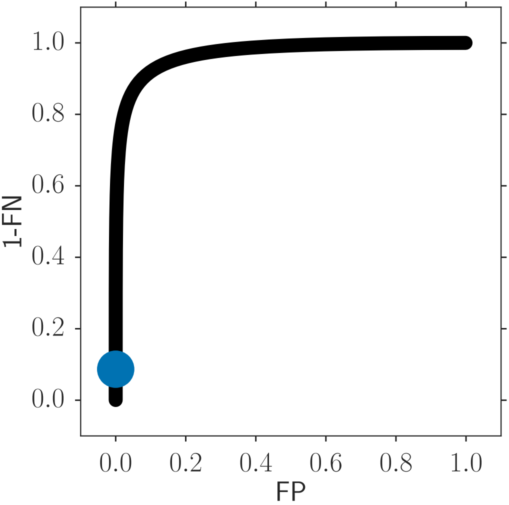

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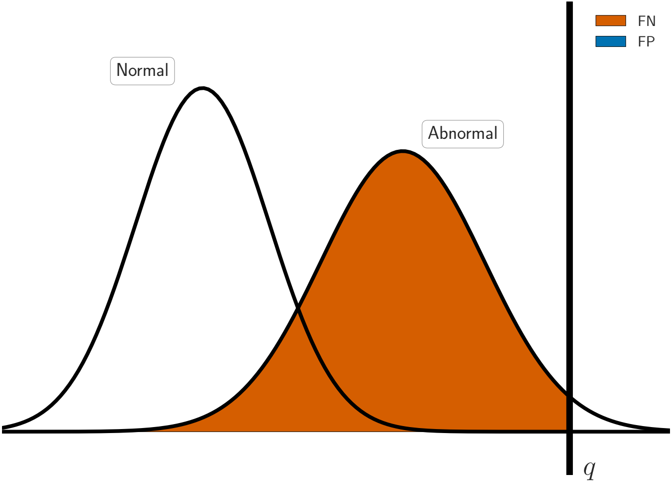

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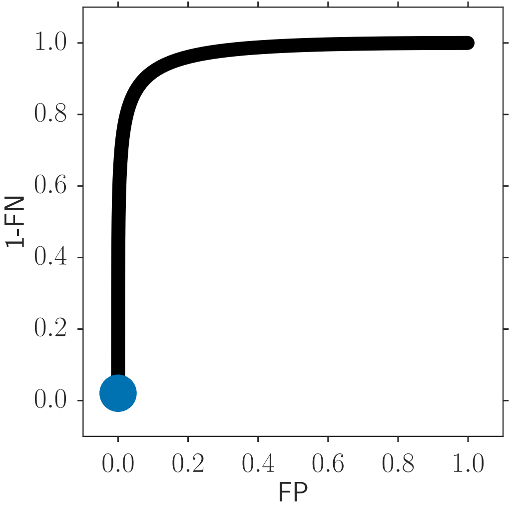


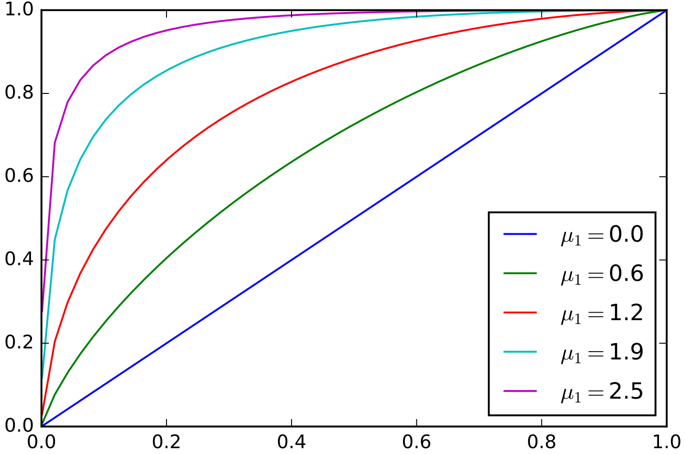
1. Statistical hypothesis testing

2. Illustration: forward variable selection

3. ROC Curve
   Presentation
   Examples

ROC curves for bi-normal case

- F and G are Gaussian with parameter μ_0, σ_0 and μ_1, σ_1, respectively.
- Here $\mu_0 = 0$, $\sigma_0 = \sigma_1 = 1$, and μ_1 varies



Estimation–application

ROC curve estimation

- Maximum likelihood
- Non-parametric
- Bayesian with latent variables
- Estimation of the area under the ROC curve (AUC)

Application

- To compare different statistic tests
- To compare different (supervised) learning algorithm
- To compare variable selection methods (*e.g.* Lasso, OMP, etc.)

nb: ROC = Receiver Operating Characteristic

References I

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