Review of Statistics

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Master MVA

Outline

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Statistical concepts

Expectation and Variances

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- Variance decomposition

Independence concepts

Independence: $X \perp\!\!\!\perp Y$

We will say that X and Y are independent and write $X \perp\!\!\!\perp Y$ iff:

$$\forall x, y, \qquad P(X = x, Y = y) = P(X = x)\, P(Y = y)$$

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Conditional Independence: $X \perp\!\!\!\perp Y \mid Z$

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- write $X \perp\!\!\!\perp Y \mid Z$ ssi:

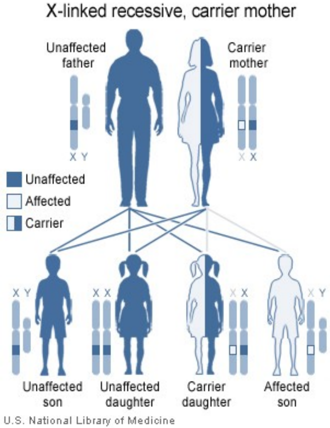
$\forall x, y, z,$

$$P(X = x, Y = y \mid Z = z) = P(X = x|Z = z)\, P(Y = y|Z = z)$$

Conditional Independence exemple

Example of
"X-linked recessive inheritance":

Transmission of the gene
responsible for hemophilia



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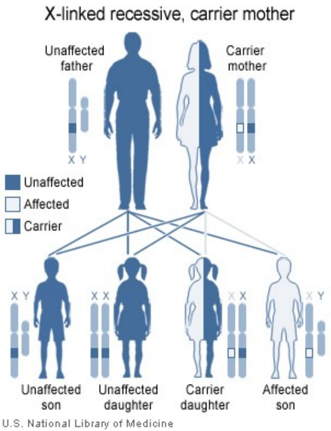

Risk for sons from an unaffected father:

- dependance between the situation of the two brothers.
- conditionally independent given that the mother is a carrier of the gene or not.

Statistical Model

Parametric model – Definition:

Set of distributions parametrized by a vector $\theta \in \Theta \subset \mathbb{R}^p$

$$\mathcal{P}_\Theta = \left\{ p_\theta(x) \mid \theta \in \Theta \right\}$$

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Multinomial model: $X \sim \mathcal{M}(n, \pi_1, \pi_2, \ldots, \pi_K) \qquad \Theta = [0, 1]^K$

$$p_\theta(x) = \binom{n}{x_1, \ldots, x_k} {\pi_1}^{x_1} \ \ldots \ {\pi_k}^{x_k}$$

Indicator variable coding for multinomial variables

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$$\mathbb{P}(C = k) = \mathbb{P}(Y_k = 1) \quad \text{and} \quad \mathbb{P}(Y = y) = \prod_{k=1}^{K} \pi_k^{y_k}.$$

Bernoulli, Binomial, Multinomial

$Y \sim \text{Ber}(\pi)$	$(Y_1, \ldots, Y_K) \sim \mathcal{M}(1, \pi_1, \ldots, \pi_K)$
$p(y) = \pi^y (1-\pi)^{1-y}$	$p(\mathbf{y}) = \pi_1^{y_1} \ldots \pi_K^{y_K}$
$N_1 \sim \text{Bin}(n, \pi)$	$(N_1, \ldots, N_K) \sim \mathcal{M}(n, \pi_1, \ldots, \pi_K)$
$p(n_1) = \binom{n}{n_1} \pi^{n_1} (1-\pi)^{n-n_1}$	$p(\mathbf{n}) = \begin{pmatrix} & n & \\ n_1 & \ldots & n_K \end{pmatrix} \pi_1^{n_1} \ldots \pi_K^{n_K}$

with

$$\binom{n}{i} = \frac{n!}{(n-i)!i!} \quad \text{and} \quad \begin{pmatrix} & n & \\ n_1 & \ldots & n_K \end{pmatrix} = \frac{n!}{n_1! \ldots n_K!}$$

Gaussian model

Scalar Gaussian model : $X \sim \mathcal{N}\left(\mu, \sigma^2\right)$

X real valued r.v., and $\theta = \left(\mu, \sigma^2\right) \in \Theta = \mathbb{R} \times \mathbb{R}_+^*$.

$$p_{\mu,\sigma^2}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right)$$

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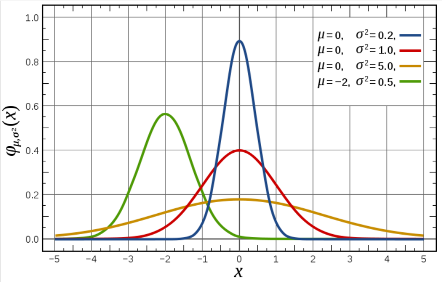
Multivariate Gaussian model: $X \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

X r.v. taking values in $\mathbb{R}^d$. If $\mathcal{K}_d$ is the set of positive definite matrices of size $d \times d$, and $\theta = (\boldsymbol{\mu}, \boldsymbol{\Sigma}) \in \Theta = \mathbb{R}^d \times \mathcal{K}_d$.

$$p_{\boldsymbol{\mu},\boldsymbol{\Sigma}}(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^d \det \boldsymbol{\Sigma}}} \exp\left(-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right)$$

Gaussian densities



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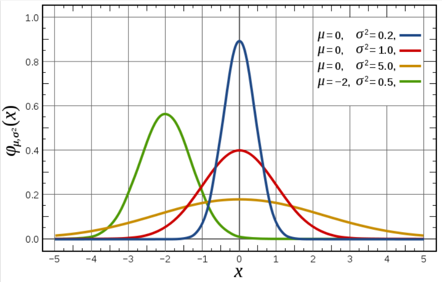

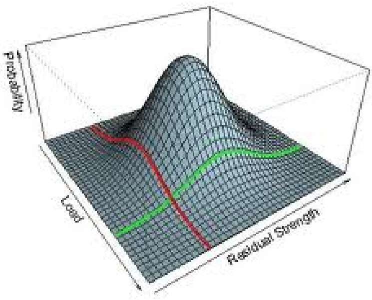

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The data used to learn or estimate a model typically consists of a collection of observation which can be thought of as instantiations of random variables.

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This collection of observations is called

- the *sample* or the *observations* in statistics
- the *sample***s** in engineering
- the *training set* in machine learning

Outline

The maximum likelihood principle

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- Let $\mathcal{P}_\Theta = \left\{ p(x;\theta) \mid \theta \in \Theta \right\}$ be a *model*
- Let x be an observation

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$$\hat{\theta}_{\mathrm{ML}} = \underset{\theta \in \Theta}{\operatorname{argmax}}\, p(x;\theta)$$

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Case of i.i.d data

If $(x_i)_{1 \le i \le n}$ is an i.i.d. sample of size n:

$$\hat{\theta}_{\mathrm{ML}} = \operatorname*{argmax}_{\theta \in \Theta} \prod_{i=1}^{n} p_\theta(x_i) = \operatorname*{argmax}_{\theta \in \Theta} \sum_{i=1}^{n} \log\ p_\theta(x_i)$$

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Thus

$$\hat{\theta}_{\mathrm{ML}} = \frac{N}{n} = \frac{x_1 + x_2 + \cdots + x_n}{n}.$$

MLE for the multinomial

Done on the board.

Outline

Method of moments (Karl Pearson, 1894)

Consider a statistical model for a *univariate* r.v. parameterized by

$$\boldsymbol{\theta} = (\theta_1, \ldots, \theta_K) \in \mathbb{R}^k.$$

Denote by μ^k the kth moment of a random variable:

$$\mu_1(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[X], \quad \mu_2(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[X^2], \quad \ldots, \quad \mu_K(\boldsymbol{\theta}) = \mathbb{E}_{\boldsymbol{\theta}}[X^K].$$

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Principle of the method of moments

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- The moment estimator is $\hat{\boldsymbol{\theta}}$ defined as the solution to the equation

$$(\hat{\mu}_1, \ldots, \hat{\mu}_K) = f(\hat{\theta}_1, \ldots, \hat{\theta}_K).$$

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$\mu_1 = \mathbb{E}[X] = \lambda p, \qquad \mu_2 = \mathbb{E}[X^2] = p(p+1)\lambda^2$, So that

$$\lambda = \frac{\mu_1^2}{\mu_2 - \mu_1^2}, \qquad p = \frac{\mu_2 - \mu_1^2}{\mu_1},$$

which yields the moment estimators

$$\hat{\lambda} = \frac{\hat{\mu}_1^2}{\hat{\mu}_2 - \hat{\mu}_1^2}, \qquad p = \frac{\hat{\mu}_2 - \hat{\mu}_1^2}{\hat{\mu}_1}.$$

Outline

Linear regression

Design matrix

Consider a finite collection of vectors $x_i \in \mathbb{R}^d$ pour $i = 1 \ldots n$.

Design Matrix

$$X = \begin{bmatrix} \text{---} & x_1^\top & \text{---} \\ \vdots & \vdots & \vdots \\ \text{---} & x_n^\top & \text{---} \end{bmatrix}.$$

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Consider a finite collection of vectors $x_i \in \mathbb{R}^d$ pour $i = 1 \dots n$.

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If x_i are not centered the design matrix of centered data can be constructed with the rows $x_i - \bar{x}^\top$ with $\bar{x} = \frac{1}{n}\sum_{i=1}^n x_i$.

Linear regression

- We consider the OLS regression for the linear hypothesis space.
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with

- the vector of outputs $\boldsymbol{y}^\top = (y_1, \dots, y_n) \in \mathbb{R}^n$
- the design matrix $\boldsymbol{X} \in \mathbb{R}^{n \times p}$ whose ith row is equal to $\mathbf{x}_i^\top$.

Solving linear regression

To solve $\min_{\boldsymbol{w} \in \mathbb{R}^p} \widehat{\mathcal{R}}_n(f_{\boldsymbol{w}})$, we consider that

$$\widehat{\mathcal{R}}_n(f_w) = \frac{1}{2n}\left(\boldsymbol{w}^\top \boldsymbol{X}^\top \boldsymbol{X} \boldsymbol{w} - 2\, \boldsymbol{w}^\top \boldsymbol{X}^\top \boldsymbol{y} + \|\boldsymbol{y}\|^2\right)$$

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Problem: $\boldsymbol{X}^\top \boldsymbol{X}$ is never invertible for $p > n$ and thus the solution is not unique.

Ridge regression

Is obtained by applying Tikhonov regularization to OLS regression.

$$\min_{\boldsymbol{w} \in \mathbb{R}^p} \frac{1}{2n} \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}\|_2^2 + \lambda \|\boldsymbol{w}\|_2^2$$

- Problem now strongly convex thus well-posed

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$\Rightarrow$ Problem now easier to solve computationally

Outline

Bayesian estimation

Bayesians treat the parameter θ as a random variable.

A priori

The Bayesian has to specify an *a priori* distribution $p(\theta)$ for the model parameters θ, which models his prior belief of the relative plausibility of different values of the parameter.

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A posteriori

The observation contribute through the likelihood: $p(x|\theta)$.
The *a posteriori* distribution on the parameters is then

$$p(\theta|x) = \frac{p(x|\theta)\,p(\theta)}{p(x)} \propto p(x|\theta)\,p(\theta)\,.$$

→ The Bayesian estimator is therefore a probability distribution on the parameters.

This estimation procedure is called Bayesian inference.

Dirichlet distribution

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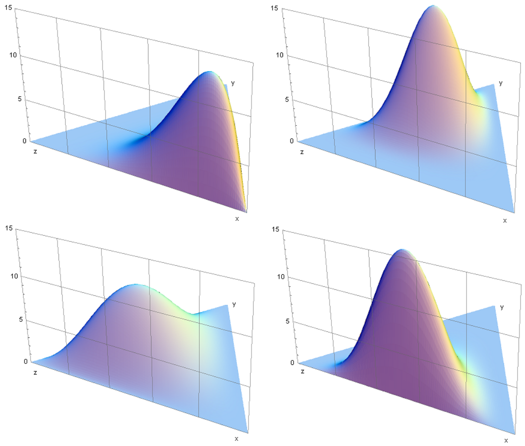
for $\boldsymbol{\theta}$ in the simplex $\triangle_K = \{\boldsymbol{u} \in \mathbb{R}_+^K \mid \sum_{k=1}^K u_k = 1\}$ and admitting the density

$$p(\boldsymbol{\theta}; \boldsymbol{\alpha}) = \frac{\Gamma(\alpha_0)}{\prod_k \Gamma(\alpha_k)} \, \theta_1^{\alpha_1 - 1} \ldots \theta_K^{\alpha_K - 1}$$

with respect to the uniform measure on the simplex, where

$$\alpha_0 = \sum_k \alpha_k \quad \text{and} \quad \Gamma(x) := \int_0^\infty t^{x-1} e^{-t} dt$$

Dirichlet distribution II



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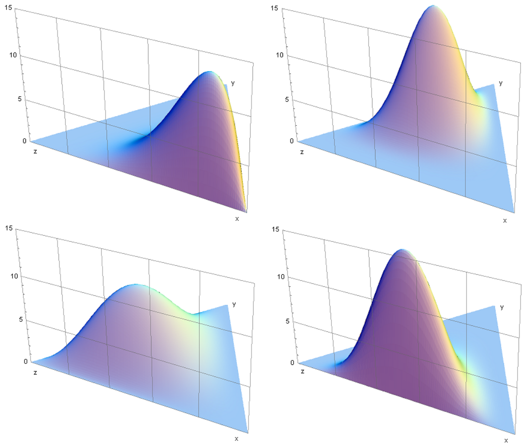

$$\mathbb{E}[\theta_k] = \frac{\alpha_k}{\alpha_0} \quad , \quad \mathrm{Var}(\theta_k) = \frac{\alpha_k(\alpha_0 - \alpha_k)}{\alpha_0^2(\alpha_0 + 1)} \quad \text{and} \quad \mathrm{Cov}(\theta_j, \theta_k) = \frac{-\alpha_j \alpha_k}{\alpha_0^2(\alpha_0 + 1)}$$

with $\alpha_0 = \sum_k \alpha_k$.

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So that $(\theta|(Z)) \sim \text{Dir}((\alpha_1 + N_1, \ldots, \alpha_K + N_K))$ with $N_k = \sum_n z_{nk}$

Use of the posterior distribution and posterior mean

The principle of Bayesian estimation is that the prior and posterior distribution model the *uncertainty* that we have in the estimation process. As a consequence, one should always integrate over the uncertainty. So the final estimate for a function $f(\boldsymbol{\theta})$ is

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If a point estimate is needed for $\boldsymbol{\theta}$ then this should be the posterior mean

$$\hat{\boldsymbol{\theta}}_{\mathrm{PM}} = \mathbb{E}\big[\boldsymbol{\theta}|\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)}\big] = \int \boldsymbol{\theta}\, p(\boldsymbol{\theta}|\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(n)})\, d\boldsymbol{\theta}$$

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Often, it is too hard or too costly to compute the **posterior mean**

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&= \arg\max_{\boldsymbol{\theta}} \sum_{i=1}^{n} \log p(\mathbf{x}^{(i)}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta})
\end{aligned}$$

... corresponds to a form of regularized maximum likelihood.

Conjugate priors

A family of prior distribution

$$\mathcal{P}_A = \{p_\alpha(\theta) \mid \alpha \in A\}$$

is said to be **conjugate** to a model $\mathcal{P}_\Theta$, if, for a sample

$$X^{(1)}, \ldots, X^{(n)} \overset{\text{i.i.d.}}{\sim} p_\theta \qquad \text{with} \qquad p_\theta \in \mathcal{P}_\Theta,$$

the distribution q defined by

$$q(\theta) = p(\theta | x^{(1)}, \ldots, x^{(n)}) = \frac{p_\alpha(\theta) \prod_i p_\theta\left(x^{(i)}\right)}{\int p_\alpha(\theta) \prod_i p_\theta\left(x^{(i)}\right) d\theta}$$

is such that

$$q \in \mathcal{P}_A.$$

Outline

Principal Component Analysis (1901)

Karl Pearson (1857 - 1936)

Empirical covariance and correlation

For centered vectors :

$$\widehat{\Sigma} = \frac{1}{n} X^\top X = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^\top$$

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Another common operation is to normalize the data by dividing each column of X by its standard deviation. This leads to the empirical covariance matrix.

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Normalisation is optional...

PCA from the analysis point of view

Data vectors live in $\mathbb{R}^d$ and one seeks a direction v in $\mathbb{R}^d$ such that the variance along this direction is maximal. Or

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\begin{aligned}
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$$\begin{aligned} Var((v^\top x_i)_{i=1\dots n}) &= \frac{1}{n}\sum_{i=1}^{n}(v^\top x_i)^2 \\ &= \frac{1}{n}\sum_{i=1}^{n} v^\top x_i x_i^\top v \\ &= v^\top \Big(\frac{1}{n}\sum_{i=1}^{n} x_i x_i^\top\Big) v \\ &= v^\top \widehat{\Sigma} v \end{aligned}$$

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Solution: first eigenvectors of $\widehat{\Sigma}$ say v_1.

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Solution: This yields the second eigenvector of $\widehat{\Sigma}$ say v_2. Etc.

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The principal directions are the eigenvectors of $\widehat{\Sigma} = V\, S^2 V^\top$.

Singular value decomposition and PCA

The SVD of a matrix $X \in \mathbb{R}^{n \times p}$ with $n \leq p$ is of the form $X = USV^\top$, avec

- $U \in \mathbb{R}^{n \times n}$ an orthogonal basis of $\mathbb{R}^n$
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The reduced SVD is more often used: If r is the rank of X then $X = USV^\top$ with,

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If the diagonal of S is such that $s_1 > s_2 > \ldots > s_r > 0$ and $U_{1k} \geq 0$ for all k the reduced SVD is unique. We have that

- $U\,S^2 U^\top$ is a (compact) diagonalisation of $XX^\top$
- $V\,S^2 V^\top$ is a (compact) diagonalisation of $X^\top X$

Eckart-Young theorem

Let $X = USV^\top$ be the SVD of X.
Let

- $U_{[k]} \in \mathbb{R}^{n \times k}$ the matrix formed by the k first columns of U
- $V_{[k]} \in \mathbb{R}^{p \times k}$ the matrix formed by the k first columns of V
- $S_{[k]} \in \mathbb{R}^{k \times k}$ the diagonal matrix with the k first singular values in S

The solution of

$$\min_Z \|X - Z\|_F^2 \quad \text{s.t.} \quad \mathrm{rank}(Z) \leq k$$

is

$$Z = X_{[k]} \qquad \text{with} \quad X_{[k]} := U_{[k]} S_{[k]} V_{[k]}^\top.$$

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Find $V = [v_1, \ldots, v_k]$ s.t. x_i have low reconstruction error on span(V):

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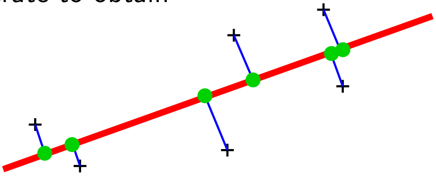

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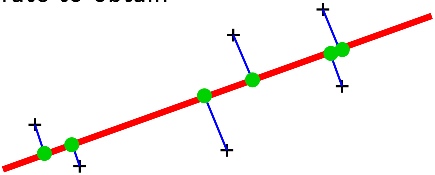

- For regular PCA, the two views are equivalent!

Outline

1. Statistical concepts
2. The maximum likelihood principle
3. Method of moments
4. Linear regression
5. Bayesian Inference
6. Principal Component Analysis
7. Mesures of performance for binary classifiers

Sensitivity, precision and co.

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Actual		"P"	"N"
	P	TP	FN
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Sensitivity, specificity, etc

	P	N
$\widehat{P}$	Sensitivity (TPR) $\frac{TP}{P}$	FPR $\frac{FP}{N}$
$\widehat{N}$	FNR $\frac{FN}{P}$	Specificity (TNR) $\frac{TN}{N}$

TPR True Positive Rate

FPR False Positive Rate

FNR False Negative Rate

NPR True Negative Rate

Precision, FDR, etc

	P	N
$\widehat{P}$	Precision (PPV) $\frac{TP}{\widehat{P}}$	FDR $\frac{FP}{\widehat{P}}$
$\widehat{N}$	FOR $\frac{FN}{\widehat{N}}$	NPV $\frac{TN}{\widehat{N}}$

PPV Positive Predictive Value

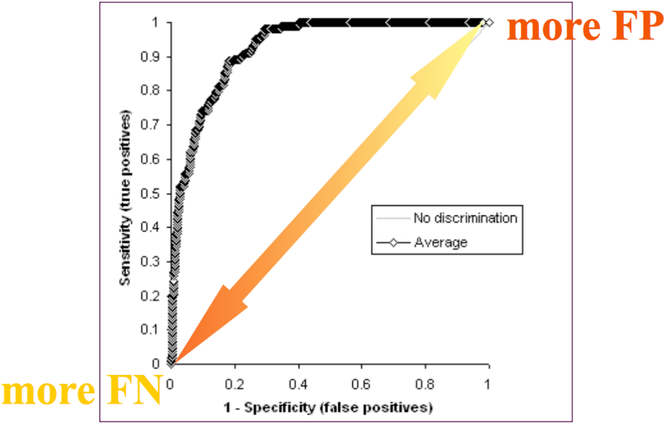
FDR False Discovery Rate

FOR False Omission Rate

NPV Negative Predictive Value

ROC curve: definition

The **Receiver Operating Characteristic** is a representation of the trade-off between r_{TP} *vs* r_{FP} as one changes the parameter controlling the sensitivity of the classifier, such as the offset b.



ROC curve: more rigorously a convex curve

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Consider the classifier c_λ that uses c_1 with probability λ and c_0 with probability $1 - \lambda$. Then

$$(\alpha_\lambda, \beta_\lambda) = \lambda(\alpha_1, \beta_1) + (1 - \lambda)(\alpha_0, \beta_0).$$

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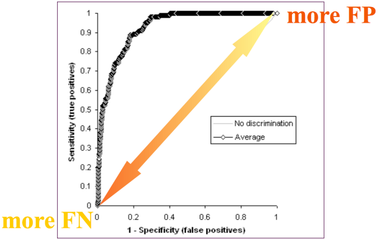

Precision Recall curve