Lecture 5

Probabilistic classifiers

Intellectual systems
(Machine Learning)

Andrey Filchenkov

04.10.2018

Lecture plan

- Bayesian classification
- Non-parametric density recovery
- Parametric density recovery
- Normal discriminant analysis
- Logistic regression

- The presentation is prepared with materials of the K.V. Vorontsov's course "Machine Leaning".
- Slides are available online: **goo.gl/BspjhF**

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Problem

An illness is spread among 1% of population. This illness test returns true answers in 95% of cases. Someone receives a positive result.

What is the probability, he actually suffers the illness?

Problem: options

An illness is spread among 1% of population. This illness test returns true answers in 95% of cases. Someone receives a positive result. What is the probability, he actually suffers the illness?

$97{,}5\% \leq x \leq 100\%$

$95\% \leq x < 97{,}5\%$

$92\% \leq x < 95\%$

$81\% \leq x < 92\%$

$70\% \leq x < 81\%$

$55\% \leq x < 70\%$

$30\% \leq x < 55\%$

$x < 30\%$

Problem: answer

An illness is spread among 1% of population. This illness test returns true answers in 95% of cases. Someone receives a positive result. What is the probability, he actually suffers the illness?

$$\Pr(d = 1|t = 1) =$$

$$= \frac{\Pr(t = 1|d = 1)\Pr(d = 1)}{\Pr(t = 1|d = 1)\Pr(d = 1) + \Pr(t = 1|d = 0)\Pr(d = 0)} =$$

$$= \frac{0.95 \times 0.01}{0.95 \times 0.01 + 0.05 \times 0.99} = \mathbf{0.16}.$$

Probabilistic classification problem

Instead of an unknown target function $y^*(x)$, we will think about an unknown probability distribution on $X \times Y$ with a density $p(x, y)$.

Simple or **independent identically distributed** (i.i.d.) sample is a sample, which contains ℓ random independent observations $T^\ell = \{(x_i, y_i)\}_{i=1}^{\ell}$.

Now we have families of distributions $\{\varphi(x, y, \theta) | \theta \in \Theta\}$ instead of algorithm models.

Problem: find an algorithm, which minimizes probability of error.

Problem statement

$a: X \to Y$ splits X on non-overlapping domains A_y:

$$A_y = \{x \in X | a(x) = y\}.$$

Error is when object x labeled as y is classified as belonging to A_s, $s \neq y$.

Error probability: $\Pr(A_s, y) = \int_{A_s} p(x, y) dx\, A_s$.

Error loss: $\lambda_{ys} \geq 0$, for all $(y, s) \in Y \times Y$.

Usually $\lambda_{yy} = 0, \lambda_y = \lambda_{ys} = \lambda_{yt}\ \forall s, t \in, s \neq y, t \neq y$.

Mean risk of a:

$$R(a) = \sum_{y \in Y} \sum_{s \in Y} \lambda_{ys} \Pr(A_s, y).$$

The main equation

$$p(X, Y) = p(x)\,\Pr(y|x) = \Pr(y)\,p(x|y)$$

$\Pr(y)$ is **priory probability** of class y.

$p(x|y)$ is **likelihood** of class y

$\Pr(y|x)$ is **posterior probability** of class y.

Two problems

First problem: **probability density recovering**

Given: $T^\ell = \{(x_i\,, y_i)\}_{i=1}^{\ell}$.

Problem: find empirical estimates $\widehat{\Pr}(y)$ and $\hat{p}(x|y)$, $y \in Y$.

Second problem: **mean risk minimization**

Given:

- prior probabilities $\Pr(y)$,
- likelihood $p(x|y), y \in Y$.

Problem: find classifier a, which minimizes $R(a)$.

Maximum a posteriori probability

Let $\Pr(y)$ and $p(x|y)$ be known for all $y \in Y$.

$$p(x, y) = p(x) \Pr(y|x) = \Pr(y)\, p(x|y).$$

Main idea: choose a class, in which the object is the most probable.

Maximum a posteriori probability (MAP):

$$a(x) = \mathrm{argmax}_{y \in Y} \Pr(y|x) = \mathrm{argmax}_{y \in Y} \Pr(y)\, p(x|y).$$

Optimal Bayesian classifier

Theorem

If $\Pr(y)$ and $p(x|y)$ are known, then the minimal mean risk $R(a)$ is achieved by Bayesian classifier

$$a_{OB}(x) = \text{argmin}_{s \in Y} \sum_{y \in Y} \lambda_{ys} \Pr(y)\, p(x|y)\,.$$

If $\lambda_{yy} = 0, \lambda_y = \lambda_{ys} = \lambda_{yt}\ \forall s, t \in Y, s \neq y, t \neq y$

$$a_{OB}(x) = \text{agrmin}_{y \in Y} \lambda_y \Pr(y)\, p(x|y).$$

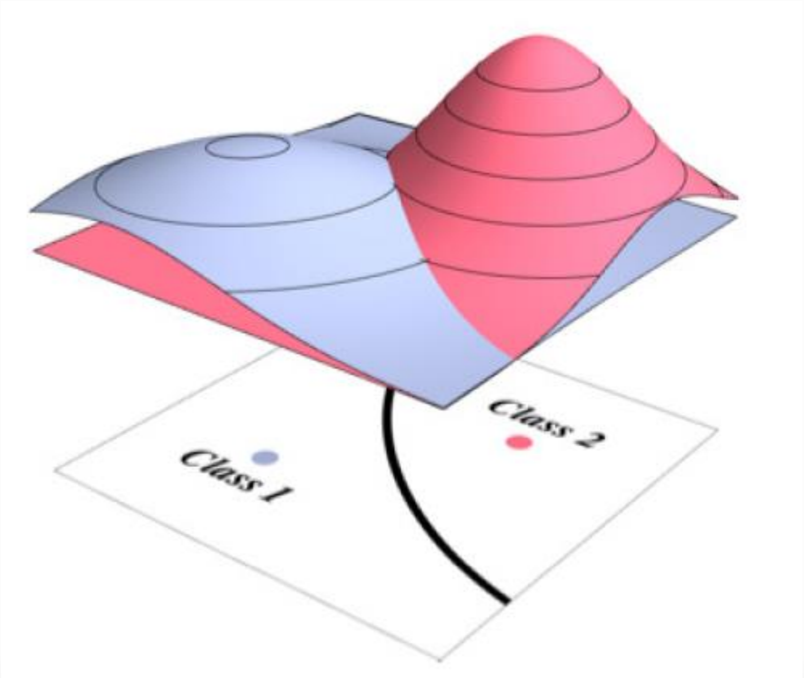
Classifier $a_{OB}(x)$ is **optimal Bayesian classifier**.

Bayesian risk is minimal value of $R(a)$.

Separating surface

Separating surface for classes a and b is locus of $x \in X$, such that maximum of Bayesian decision rule is achieved both for $y = s$ and $y = t$:

$$\lambda_a \Pr(a)\, p(x|a) = \lambda_s \Pr(b)\, p(x|b).$$



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Two subproblems

The problem is to estimate prior and posterior probabilities for each class:

$$\widehat{\Pr}(y) = ?$$
$$\hat{p}(x|y) = ?$$

The first subproblem can be solved easily:

$$\widehat{\Pr}(y) = \frac{|X_y|}{\ell}, \qquad X_y = \{x_i, y_i \in T^\ell, y_i = y\}.$$

The second one is much more complex.

Instead of recovering $(x|y)$, we will recover $p(x)$ with $T^m = \big((x_{(1)}, s), \dots, (x_{(m)}, s)\big)$ for each $s \in Y$.

One-dimensional case

If $\Pr([a,b])$ is a probabilistic measure on $[a,b]$, then

$$p(x) = \lim_{h\to 0} \frac{1}{2h} \Pr([x-h, x+h]).$$

Empirical density estimation with window of a width h

$$\widehat{p_h}(x) = \frac{1}{2mh} \sum_{i=1}^{m} [|x - x_i| < h].$$

Parzen-Rosenblatt window

Empirical density estimation with window of a width h:

$$\widehat{p_h}(x) = \frac{1}{2hm} \sum_{i=1}^{m} \left[\frac{x - x_i}{h} < 1 \right].$$

Parzen-Rosenblatt estimation for a window with width h:

$$\widehat{p_h}(x) = \frac{1}{hm} \sum_{i=1}^{m} K\left(\frac{x - x_i}{h} \right),$$

where $K(r)$ is a kernel function.

$\widehat{p_h}(x)$ converges to $p(x)$.

Generalization to multidimensional case

1. If objects are described with n numeric features $f_j \colon X \to \mathbb{R}, j = 1, \ldots, n$,

$$\widehat{p_h}(x) = \frac{1}{m} \sum_{i=1}^{m} \prod_{j=1}^{n} \frac{1}{h_j} K\left(\frac{f_j(x) - f_j(x_i)}{h_j}\right).$$

2. If X is a (metric) space with a distance $\rho(x, x')$:

$$\widehat{p_h}(x) = \frac{1}{mV(h)} \sum_{i=1}^{m} K\left(\frac{\rho(x, x_i)}{h}\right),$$

where $V(h) = \int_X K\left(\frac{\rho(x,x_i)}{h}\right) dx$ is normalizing factor.

Multidimensional Parzen window

Estimate $\widehat{p_h}(x)$ with

$$\widehat{p_h}(x) = \frac{1}{mV(h)} \sum_{i=1}^{m} K\left(\frac{\rho(x, x_i)}{h}\right),$$

Parzen window:

$$a(x; T^\ell, h) = \arg\max_{y \in Y} \lambda_y \Pr(y)\, \ell_y^{-1} \sum_{i: y_i = y} K\left(\frac{\rho(x, x_i)}{h}\right).$$

$\Gamma_y(x) = \lambda_y \Pr(y)\, \ell_y^{-1} \sum_{i: y_i = y} K\left(\frac{\rho(x, x_i)}{h}\right)$ is a closeness to class.

Naïve Bayesian classifier

Hypothesis (naïve): features are independent random variables with probability densities $p_j(\xi|y)$, $y \in Y$, $j = 1, \dots, n$.

Then classes likelihoods can be represented as:

$$p(x|y) = p_1(\xi_1|y) \cdot \ldots \cdot p_n(\xi_n|y), \qquad x = (\xi_1, \dots, \xi_n), y \in Y.$$

Naïve Bayesian classifier:

$$a(x) = \mathrm{argmax}_{y \in Y} \left(\ln \lambda_y \widehat{\Pr}(y) + \sum_{j=1}^{n} \ln \widehat{p_j}(\xi_j|y) \right).$$

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Parametrical notation

Joint probability density for sample:

$$p(T^\ell) = p\big((x_1, y_1), \dots, (x_\ell, y_\ell)\big) = \prod_{i=1}^{\ell} p(x_i, y_i).$$

Likelihood:

$$L(\theta, T^\ell) = \prod_{i=1}^{\ell} \varphi(x_i, y_i, \theta).$$

MAP:

$$a_\theta(x) = \operatorname{argmax}_y \varphi(x, y, \theta).$$

Relation with empirical risk

Find logarithm:

$$-\ln L\left(\theta, T^{\ell}\right) = -\sum_{i=1}^{\ell} \ln \varphi(x_i, y_i, \theta) \to \min_{\theta}.$$

Define loss function:

$$L(a_{\theta}, x) = -\ell \ln \varphi(x, y, \theta).$$

Then empirical risk minimization problem is:

$$Q\left(a_{\theta}, T^{\ell}\right) = \frac{1}{\ell}\sum\nolimits_{1}^{\ell} L(a_{\theta}, x) =$$

$$= -\frac{1}{\ell}\sum\nolimits_{1}^{\ell} \ell \ln \varphi(x, y, \theta) = -\sum_{i=1}^{\ell} \ln \varphi(x_i, y_i, \theta) \to \min_{\theta}.$$

Maximum likelihood

Principle of **maximum likelihood**:

$$L(\theta; X^m) = \sum_{i=1}^{m} \ln \varphi(x_i; \theta) \to \max_\theta,$$

Optimum for θ is achieved in a point, in which the derivate value is zero.

Principle of maximum weighted likelihood:

$$L(\theta; X^m, W^m) = \sum_{i=1}^{m} w_i \ln \varphi(x_i; \theta) \to \max_\theta,$$

where $W^m = \{w_1, \dots, w_m\}$ is a vector of object weights.

Maximum joint likelihood principle

$$Q(a_\theta, T^\ell) = -\sum_{i=1}^{\ell} \ln \varphi(x_i, y_i, \theta) \to \min_\theta .$$

$$\varphi(x_i, y_i, \theta) = p(x_i, y_i | w) p(w, \gamma),$$

$p(x_i, y_i | w)$ is a probabilistic data model, $p(w, \gamma)$ is prior distribution of model parameters, γ is hyper-parameter.

Maximum joint likelihood principle:

$$\sum_{i=1}^{\ell} \ln p(x_i, y_i | w) + \ln p(w, \gamma) \to \max_{w,\gamma} .$$

Quadratic penalty conditions

Let $w \in \mathbb{R}^n$ is described with n-dimensional Gaussian distribution:

$$p(w;\sigma) = \frac{1}{(2\pi\sigma)^{n/2}} \exp\left(-\frac{\|w\|^2}{2\sigma}\right),$$

(weights are independent, their expectations are equal to zeros, their variances are the same and equal to σ).

It leads to quadratic penalty:

$$-\ln p(w;\sigma) = \frac{1}{2\sigma}\|w\|^2 + \mathrm{const}(w).$$

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Key hypothesis

Key hypothesis: classes have n-dimensional normal densities:

$$p(x|y) = \mathcal{N}\left(x; \mu_y, \Sigma_y\right) = \frac{e^{-\frac{1}{2}(x-\mu_y)^\top \Sigma_y^{-1}(x-\mu_y)}}{\sqrt{(2\pi)^n \det \Sigma_y}},$$

where μ_y is vector of expectation of class $y \in Y$,

$\Sigma_y \in \mathbb{R}^{n\times n}$ is covariance matrix for class $y \in Y$,

it is symmetrical, nonsingular, positive define matrix.

Theorem on separating surface

Theorem:

If classes densities are normal

1) separating surface
$$\{x \in X | \lambda_y \Pr(y)\, p(x|y) = \lambda_s \Pr(s)\, p(x|s)\}$$
is quadratic;
2) if $\Sigma_{y_+} = \Sigma_{y_-}$, then it is linear.

Quadratic analysis

Principle of maximum weighted likelihood:

$$L(\theta; X^m, W^m) = \sum_{i=1}^{m} w_i \ln \varphi(x_i; \theta) \to \max_\theta,$$

where $W^m = \{w_1, \ldots, w_m\}$ is vector of object weights.

Optimum for θ is achieved in point where derivate value is zero.

Quadratic discriminant

Theorem:

Estimates for maximum weighed likelihood with $y \in Y$ are:

$$\widehat{\mu_y} = \frac{1}{W_y} \sum_{y:y_i=y} w_i x_i;$$

$$\widehat{\Sigma_y} = \frac{1}{W_y} \sum_{y:y_i=y} w_i \left(x - \widehat{\mu_y}\right)\left(x - \widehat{\mu_y}\right)^\top;$$

where $W_y = \sum_{y:y_i=y} w_i$.

Quadratic discriminant:

$$a(x) = \mathrm{argmax}_{y \in Y} \left(\ln \lambda_y \Pr(y) - \frac{1}{2}\left(x - \widehat{\mu_y}\right)^\top \Sigma_y^{-1} \left(x - \widehat{\mu_y}\right) - \frac{1}{2} \ln \det \widehat{\Sigma_y} \right).$$

Method problems

- If $\ell_y < n$, then $\widehat{\Sigma_y}$ is singular.
- The less ℓ_y is, the less $\widehat{\Sigma_y}$ is robust.
- Estimates $\widehat{\mu_y}$ and $\widehat{\Sigma_y}$ are sensitive to noise.
- Distributions are required to be normal.

Linear discriminant analysis

Hypothesis: covariance matrices are equal

$$\hat{\Sigma} = \frac{1}{W_y} \sum_{y:y_i=y} w_i \left(x - \widehat{\mu_{y_i}}\right)\left(x - \widehat{\mu_{y_i}}\right)^\top.$$

Fisher's linear discriminant:

$$a(x) = \operatorname{argmax}_{y \in Y} \Big(\lambda_y \Pr(y)\, p(x|y)\Big) =$$

$$= \operatorname{argmax}_{y \in Y} \left(\ln \lambda_y \widehat{\Pr(y)} - \frac{1}{2} \widehat{\mu_y}^\top \hat{\Sigma}^{-1} \widehat{\mu_y} - x^\top \hat{\Sigma}^{-1} \widehat{\mu_y}\right) =$$

$$= \operatorname{argmax}_{y \in Y} \left(\beta_y + x^\top \alpha_y\right) = \operatorname{sign}(\langle x, w \rangle - w_0).$$

Mahalanobis distance

Theorem: error probability of Fisher's linear discriminant equals

$$R(a) = \Phi\left(-\frac{1}{2}\|\mu_1 - \mu_2\|_\Sigma\right),$$

where $\Phi(r) = \mathcal{N}(x; 0,1)$.

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Bayesian classification

A distribution $p(x, y)$ on object-answers space.

Simple sample of size ℓ

$$T^\ell = \{(x_i, y_i)\}_{i=1}^{\ell}.$$

Bayesian classifier:

$$a_{OB}(x) = \text{argmax}_{y \in Y} \lambda_y \Pr(y)\, p(x|y),$$

where λ_y is losses for class y.

Linear classifiers

Constraint: $Y = \{-1, +1\} = \{y_{-1}, y_{+1}\}$

Linear classifier:

$$a_w(x, T^\ell) = \mathrm{sign}\left(\sum_{i=1}^{n} w_i f_i(x) - w_0\right).$$

where $w_1, \dots, w_n \in \mathbb{R}$ are features weights.

$$a_w(x, T^\ell) = \mathrm{sign}(\langle w, x \rangle).$$

Linear Bayesian classifiers

$$Q(a_\theta, T^\ell) = \frac{1}{\ell}\sum\nolimits_1^\ell L(a_\theta, x) = -\sum_{i=1}^{\ell} \ln \varphi(x_i, y_i, \theta) \to \min_\theta .$$

Bayesian classifier for two classes:

$$a(x) = \operatorname{sign}(\lambda_+ \Pr(y_+|x) - \lambda_- \Pr(y_- |x)) =$$

$$= \operatorname{sign}\left(\frac{p(x|y_+)}{p(x|y_-)} - \frac{\lambda_- \Pr(y_-)}{\lambda_+ \Pr(y_+)}\right).$$

Separating surface

$$\lambda_+ \Pr(y_+) p(x|y_+) = \lambda_- \Pr(y_-) p(x|y_-)$$

is linear.

Key hypothesis

Key hypothesis: classes are defined with n-dimensional overdispersed exponential densities:

$$p(x|y) = \exp\left(c_y(\delta)\langle\theta_y, x\rangle + b_y(\delta, \theta_y) + d(x, \delta)\right),$$

where $\theta_y \in \mathbb{R}^m$ is **shift** parameter,

δ is **dispersion** parameter**;**

b_y, c_y, d are some numeric functions.

Overdispersed exponential distribution family includes:

uniform, normal, hypergeometric, Poisson, binominal, Γ-distribution and other.

Example: Gaussian

Let $\theta = \Sigma^{-1}\mu;\ \delta = \Sigma.$

Then

$$\mathcal{N}(x;\mu,\Sigma) = \frac{e^{-\frac{1}{2}(x-\mu)^\top\Sigma^{-1}(x-\mu)}}{\sqrt{(2\pi)^n \det\Sigma}} =$$

$$= \exp\left(\left(\mu^\top\Sigma^{-1}x\right) - \left(\frac{1}{2}\mu^\top\Sigma^{-1}\Sigma\Sigma^{-1}\mu\right)\right.$$

$$\left. - \left(\frac{1}{2}x^\top\Sigma^{-1}x + \frac{n}{2}\ln 2\pi + \frac{1}{2}\ln|\Sigma|\right)\right).$$

The main theorem

Theorem:

If p_y are overdispersed exponential distributions and $f_0(x) = \text{const}$, then

1) Bayesian classifier

$$a(x) = \text{sign}\left(\frac{p(x|y_+)}{p(x|y_-)} - \frac{\lambda_- \Pr(y_-)}{\lambda_+ \Pr(y_+)}\right)$$

is linear: $a(x) = \text{sign}(\langle w, x\rangle - w_0),\ w_0 = \ln\frac{\lambda_-}{\lambda_+}$;

2) posterior probabilities of classes are:

$$\Pr(y|x) = \sigma(\langle w, x\rangle y),$$

where $\sigma(s) = \frac{1}{1+e^{-s}}$, which is **logistic (sigmoid) function**.

Logarithmic loss function

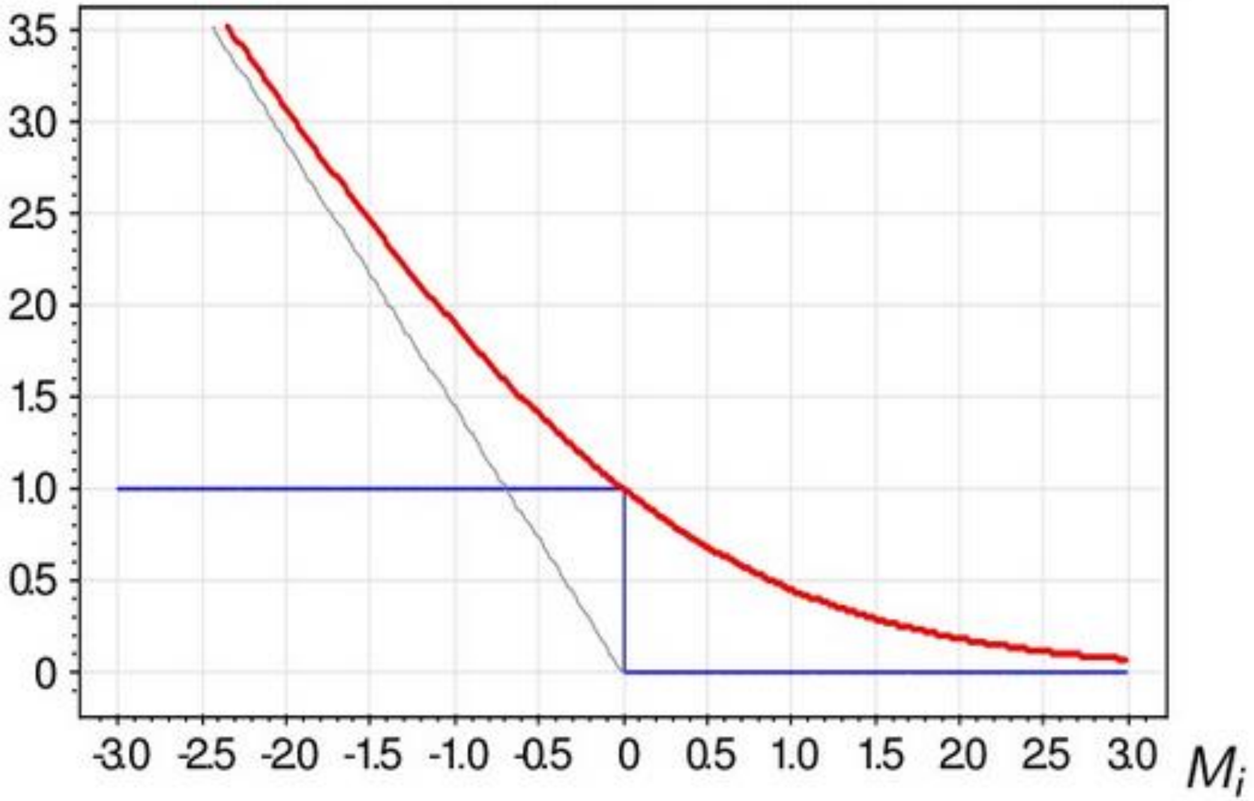
$$\widetilde{Q_w}(a, T^\ell) = \sum_i^\ell L(a, x_i) = \sum_i^\ell \ln p(x_i, y_i; w)$$

$$p(x, y; w) = \Pr(y|x)p(x) = \sigma(\langle w, x\rangle y)\text{const}(w)$$

$$\widetilde{Q_w}(a, T^\ell) = \sum_i^\ell \ln(1 + \exp(-\langle w, x\rangle y)) \to \min_w.$$

That is logarithmic loss function.

Logarithmic loss function plot



Gradient descent

Derivative:

$$\sigma'(s) = \sigma(s)\sigma(-s).$$

Gradient:

$$\mu\nabla\tilde{Q}\left(w^{[k]}\right) = -\sum_{i}^{\ell} y_i x_i \sigma\left(-M_i(w)\right).$$

Gradient descent step:

$$w^{[k+1]} = w^{[k]} - \mu y_i x_i \sigma\left(-M_i\left(w^{[k]}\right)\right).$$