Lecture 3

Linear methods

Intellectual system
(Machine Learning)

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Lecture plan

- Linear classification
- Gradient descent
- Linear regression and matrix decomposition
- Regularization

- 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 formulation

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

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

Find classifier $a_w\left(x, T^{\ell}\right) = \text{sign}\left(f(x, w)\right)$.

$f(x, w)$ is a discernment function,

w is a parameter vector.

Key hypothesis: objects are (well-)separable.

Main idea: search among separating surfaces described with $f(x, w) = 0$.

Margin

Margin of object x_i:

$$M_i(w) = y_i f(x_i, w),$$

$M_i(w) < 0$ is an evidence of misclassification.

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We have previously defined **margin** of object x_i as

$$M(x_i) = C_{y_i}(x_i) - \max_{y \in Y \setminus \{y_i\}} C_y(x_i),$$

where $C_y(u) = \sum_{i=1}^{\ell} [y(u,i) = y] w(i,u)$, $w(i,u)$ is function of u's ith neighbor importance.

What is their relation?

Loss function smoothing

Empirical risk:

$$Q\left(a_w, T^\ell\right) = Q(w) = \sum_i^\ell [M_i(w) < 0],$$

it is just the number of errors.

The function is not smooth, so it is hard to find optima.

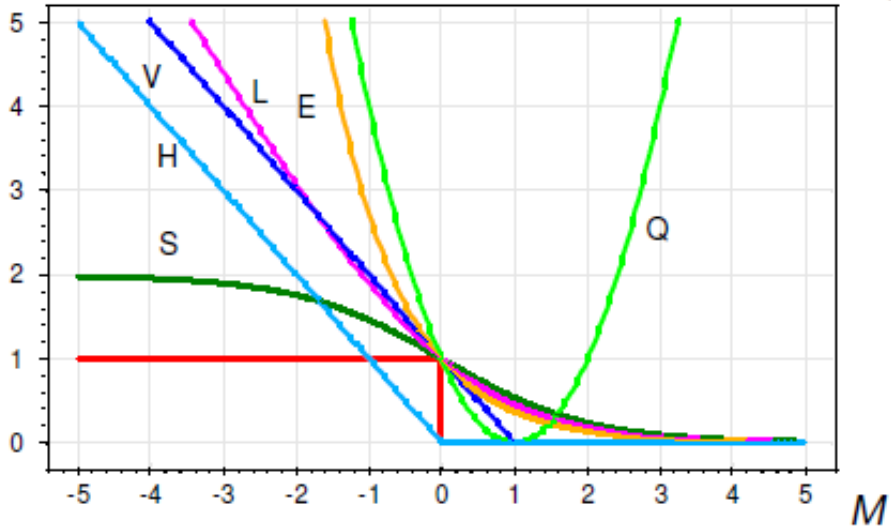
Approximation:

$$\tilde{Q}(w) = \sum_i^\ell L(M_i(w)),$$

where $L\left(M_i(w)\right) = L(a_w\left(x_i, T^\ell\right), x_i)$ is a loss function.

Smooth loss functions

We want L to be non-negative, non-increasing, and smooth:



$H(M) = (-M)_+$ — piecewise linear (Hebb's rule);
$V(M) = (1 - M)_+$ — piecewise linear (SVM);
$L(M) = \log_2(1 + e^{-M})$ — logarithmic (LR);
$Q(M) = (1 - M)^2$ — square (LDA);
$S(M) = 2(1 + e^{M})^{-1}$ — sigmoid (ANN);
$E(M) = e^{-M}$ — exponential (AdaBoost).

Linear classifier

$f_j: X \to \mathbb{R}, j = 1, \ldots, n$ are numeric features.

Linear classifier:

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

$w_1, \ldots w_n \in \mathbb{R}$ are feature **weights**.

Equivalent notation:

$$a_w\left(x, T^\ell\right) = \text{sign}(\langle w, x \rangle),$$

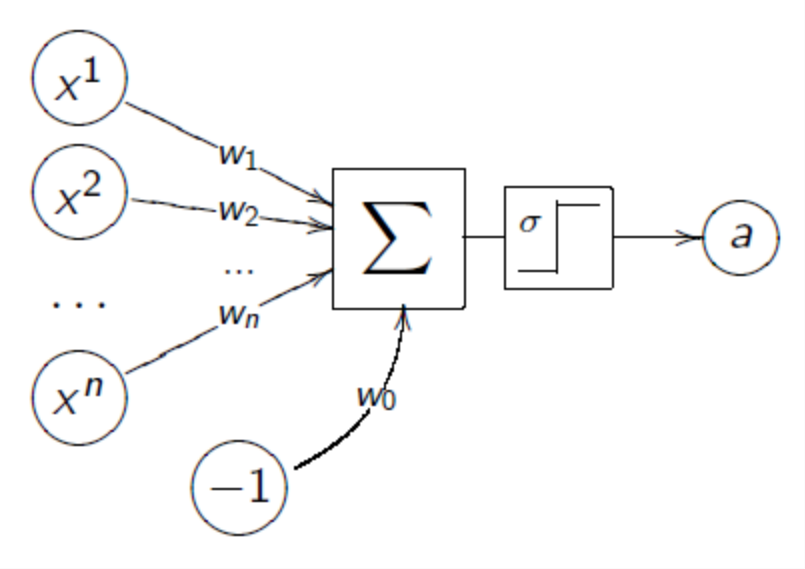
if a feature $f_0(x) = -1$ is added.

Neuron

McCulloch-Pitts neuron:

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

where σ is an activation function.



How to learn a linear classifier?

We have to choose parameter vector w.

We can use almost any optimization algorithm capable to optimize empirical risk in the corresponding space.

The empirical risk is not black-box function.

Even more, we have guaranteed that it is a smooth function.

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Gradient descent

Empirical risk minimization problem

$$\tilde{Q}(w) = \sum_{i}^{\ell} L\big(M_i(w)\big) = \sum_{i}^{\ell} L(\langle w, x_i\rangle y_i) \to \min_w.$$

Gradient descent (a.k.a Batch gradient descent):

$w^{[0]} =$ **an initial guess value**;

$w^{[k+1]} = w^{[k]} - \mu \nabla Q\big(w^{[k]}\big)$,

where μ is a **gradient step** a.k.a **learning rate.**

$$w^{[k+1]} = w^{[k]} - \mu \sum_i^{\ell} L'(\langle w, x_i\rangle y_i)\, x_i y_i.$$

Stochastic gradient descent

Problem is that there are too many objects, which should be estimated on each step.

Stochastic gradient descent:

$w^{[0]}$ is **an initial guess values**;

$x_{(1)}, \ldots, x_{(\ell)}$ is **an objects order**;

$$w^{[k+1]} = w^{[k]} - \mu L'\left(\langle w^{[k]}, x_{(k)}\rangle y_{(k)}\right),$$

$$Q^{[k+1]} = (1-\alpha)Q^{[k]} + \alpha L\left(\langle w^{[k]}, x_{(k)}\rangle y_{(k)}\right).$$

Stop when values of Q and/or w do not change much.

Mini-batch gradient descent

Problem is that it is a bit too random because it depends only on a single object.

Mini-batch gradient descent:

$w^{[0]}$ is **an initial guess values**; b is **batch size**

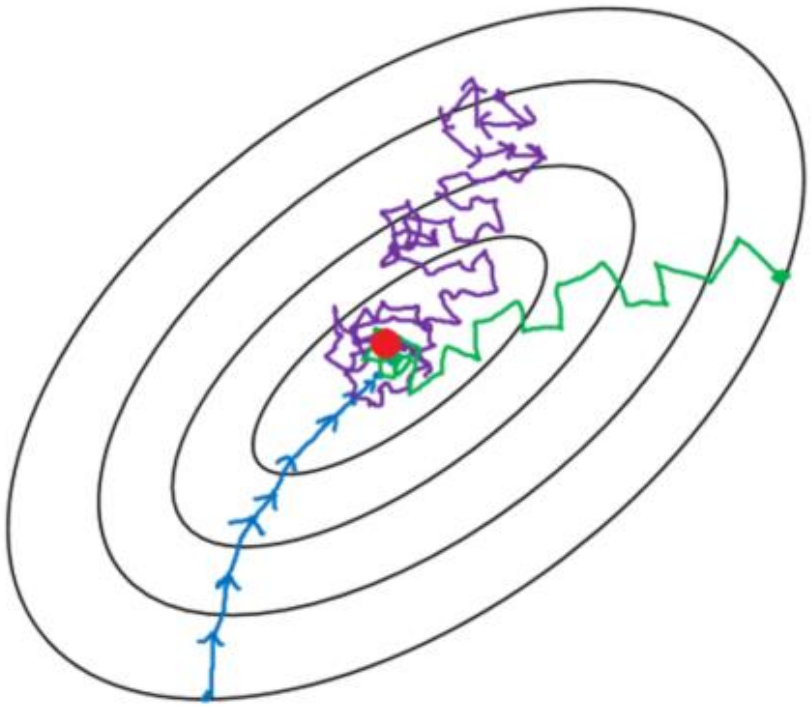
$x_{(1)}, \dots, x_{(\ell)}$ is **an objects order**;

$$w^{[K+1]} = w^{[K]} - \mu \sum_{k=Kb}^{k=(K+1)b} L'\left(\langle w^{[k]}, x_{(k)}\rangle y_{(k)}\right),$$

$$Q^{[K+1]} = (1-\alpha)Q^{[K]} + \alpha L\left(\langle w^{[k]}, x_{(k)}\rangle y_{(k)}\right).$$

Stop when values of Q and/or w do not change much.

Comparison



Batch gradient descent
Mini-batch gradient Descent
Stochastic gradient descent

Mini-batch gradient descent

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Stop when values of Q and/or w do not change much.

Novikov's theorem

Theorem (Novikov)

Let sample T^ℓ be linearly separable: $\exists \widetilde{w}, \exists \delta > 0$:

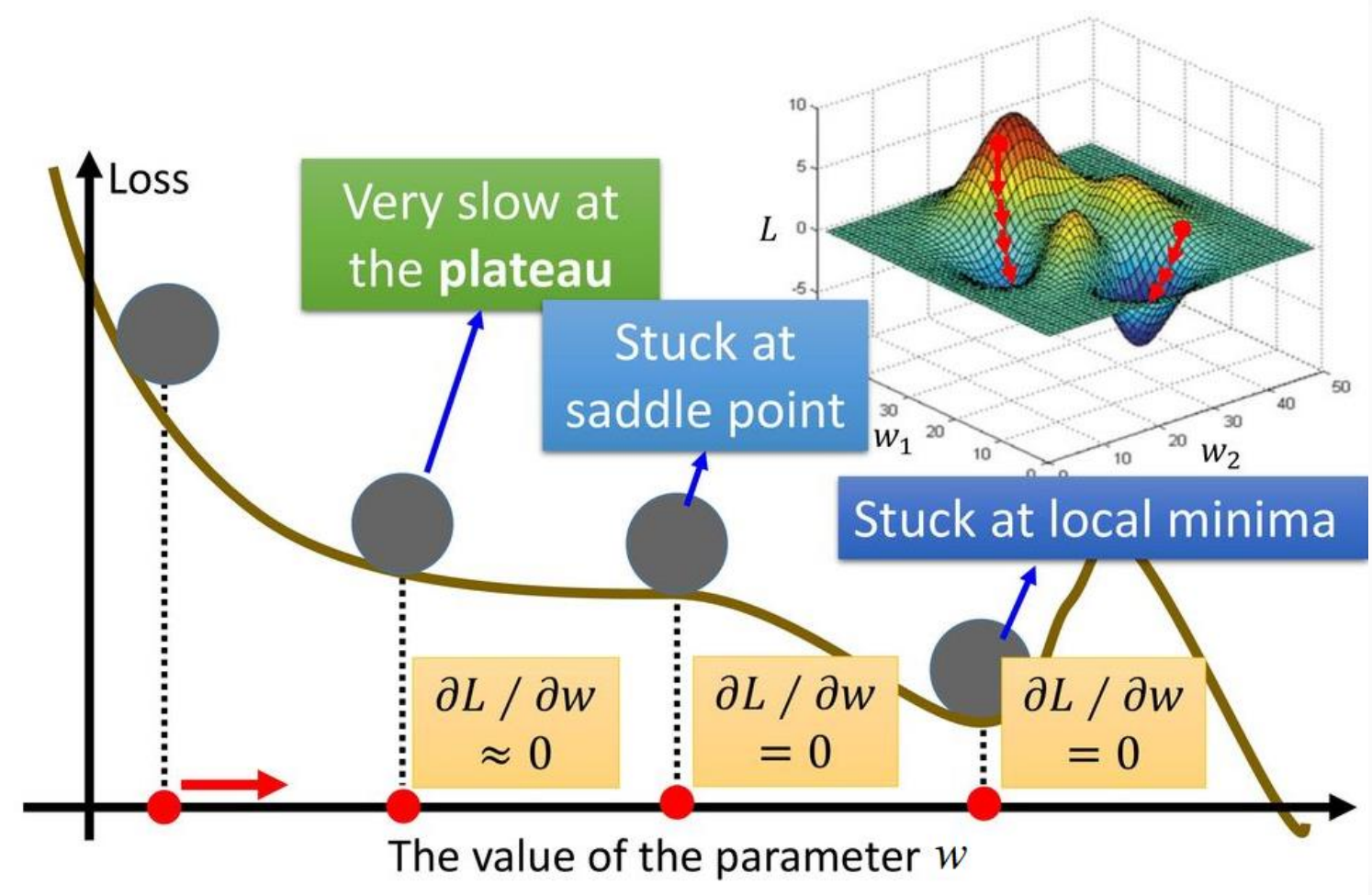
$\langle \widetilde{w}, x_i \rangle y_i > \delta$ for all $i = 1, \ldots, \ell$.

Them the stochastic gradient descent with Hebb's rule will find weight vector w, which:

- splits sample without error;
- with any initial guess $w^{[0]}$;
- with any learning rate $\mu > 0$;
- independently on objects ordering $x_{(i)}$;
- with finite numbers of changing vector w;
- if $w^{[0]} = 0$, then the number of changes in vector w is

$t_{\max} \leq \frac{1}{\delta^2} \max ||x_j||$.

Convergence problems

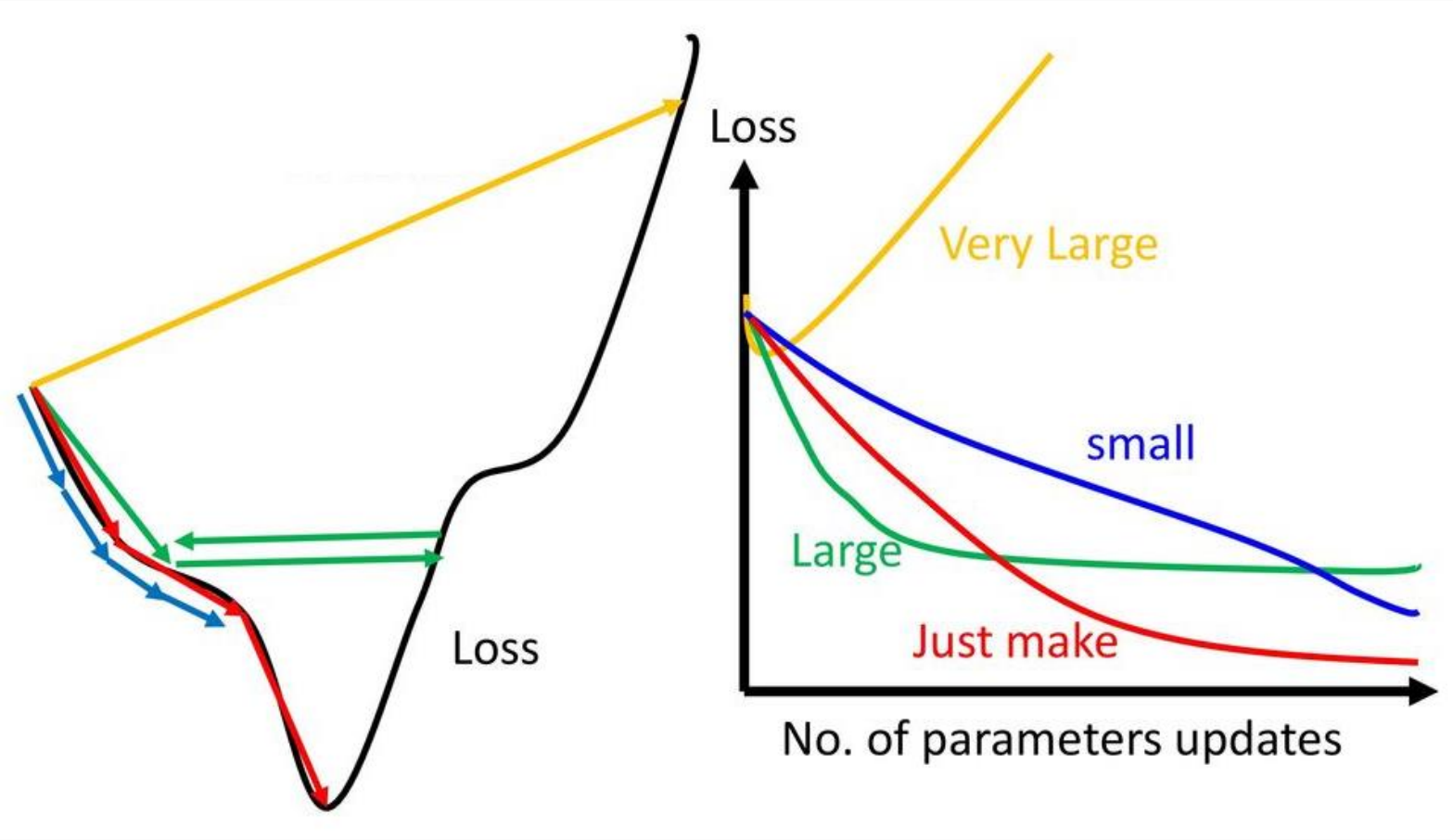


Heuristics for initial guesses

Important for non-convex functions

- $w_j = 0$ for all $j = 0, \ldots, n$;
- small random values: $w_j \in \left[-\frac{1}{2n}, \frac{1}{2n}\right]$;
- $w_j = \frac{\langle y, f_j \rangle}{\langle f_j, f_j \rangle}$;
- learn it with a small random subsample;
- multiply runs with different initial guesses.

Learning rates comparison



Heuristics for learning rate

- Convergence is achieved for convex functions when

$$\mu^{[k]} \to 0, \sum \mu^{[k]} = \infty, \sum \left(\mu^{[k]}\right)^2 < \infty.$$

- **Steepest gradient descent**:

$$Q\left(w^{[k]} - \mu^{[k]} \nabla Q\left(w^{[k]}\right)\right) \to \min_{\mu^{[k]}}.$$

- Steps for "jog of" local minima.
- Second order methods.

Heuristics for object ordering

- take objects from different classes by turns;
- take misclassified objects more frequently;
- do not take "good" object, such that $M_i > \kappa_+$;
- do not take noisy objects, such that $M_i < \kappa_-$.

SG algorithm discussion

Advantages:

- it is easy to implement;
- it is easy to generalize for any f and L;
- dynamical learning;
- can handle small samples.

Disadvantages:

- slow convergence or even divergence is possible;
- can stuck in local minima, saddle points;
- proper heuristic choice is very important;
- overfitting.

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Linear regression model

Model of multidimensional linear regression:

$$f(x,\theta)=\sum_{j=1}^{n}\theta_j f_j(x),\quad \theta\in\mathbb{R}^n.$$

Matrix notation:

$$F=\begin{pmatrix} f_1(x_1) & \dots & f_n(x_1)\\ \dots & \dots & \dots\\ f_1(x_\ell) & \dots & f_n(x_\ell)\end{pmatrix}, y=\begin{pmatrix} y_1\\ \dots\\ y_\ell\end{pmatrix}, \theta=\begin{pmatrix}\theta_1\\ \dots\\ \theta_n\end{pmatrix}.$$

Quality in matrix notation:

$$Q\left(\theta,T^\ell\right)=\sum_{i=1}^{\ell}(f(x_i,\theta)-y_i)^2=||F\theta-y||^2\to\min_{\theta\in\mathbb{R}}.$$

Matrix decomposition

There are plenty of ways how it can be solved.

One of the most popular way is to apply singular **vector** decomposition, which is a **matrix decomposition** (a.k.a. **matrix factorization**) method.

Normal equation system

Minimum condition:

$$\frac{\partial Q(\theta)}{\partial \theta} = 2F^{\top}(F\theta - y) = 0.$$

$$\theta^{*} = \left(F^{\top}F\right)^{-1}F^{\top}y$$

$F^{+} = \left(F^{\top}F\right)^{-1}F^{\top}$ is **pseudo reverse matrix** (**Moore–Penrose inverse**)

$P_F = FF^{+}$ is **projection matrix**

Solution:

$$\theta^{*} = F^{+}y.$$

Minimum approximation:

$$Q(\theta^{*}) = ||P_F y - y||^2.$$

Singular vector decomposition

Theorem: any matrix F size of $\ell \times n$ can be represented with singular decomposition

$$F = VDU^{\top}.$$

With

- $V = (v_1, \dots, v_n)$ is size of $\ell \times n$ and orthogonal $V^{\top}V = I_n$, rows v_j are eigenvectors of matrix $FF^{\top}$;
- $U = (u_1, \dots, u_n)$ is size of $n \times n$ and ortogonal $U^{\top}U = I_n$, rows u_j are eigenvectors of matrix $F^{\top}F$;
- $D = \operatorname{diag}\left(\sqrt{\lambda_1}, \dots, \sqrt{\lambda_n}\right)$ of size $n \times n$, $\sqrt{\lambda_j}$ are **singular numbers**, squares of eigenvalues of matrices $FF^{\top}$ and $F^{\top}F$.

SVD interpretation

You can think of some latent space, to which we want to project data.

D represents importance of each basis vector

V represents how objects correspond to the basis vectors

U represents how features correspond to the basis vectors

OLS with SVD

$$F^+ = \left(UDV^\top VDU^\top\right)^{-1} UDV^\top = UD^{-1}V^\top = \sum_{j=1}^{n} \frac{1}{\sqrt{\lambda_j}} u_j v_j^\top;$$

$$\theta^* = F^+ y = UD^{-1}V^\top y = \sum_{j=1}^{n} \frac{1}{\sqrt{\lambda_j}} u_j (v_j^\top y);$$

$$F\theta^* = P_F y = \left(VDU^\top\right) UD^{-1}V^\top y = VV^\top y = \sum_{j=1}^{n} v_j (v_j^\top y);$$

$$||\theta^*||^2 = ||D^{-1}V^\top y||^2 = \sum_{j=1}^{n} \frac{1}{\lambda_j} \left(v_j^\top y\right)^2.$$

Discussion

- When we can compute SVD, we can easily find solution for OLS.
- SVD is computations are quite heavy still, its complexity is $O\left(\ell^2 n + n^3\right)$

- SVD is important in many other machine learning tasks, first of all, in dimensionality reduction.

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Regularization

Key hypothesis: w "swings" during training causing overfitting

Main idea: clip w norm.

Add regularization penalty for weights norm:

$$Q_\tau\left(a_w, T^\ell\right) = Q\left(a_w, T^\ell\right) + \frac{\tau}{2}\|w\|^2 \to \min_w.$$

τ is a coefficient representing the strength of model regularization, or, equally, is a trade-off between model performance and generalizability.

Ridge regression

Assumption: values of θ have Gaussian distribution with covariance matrix σI_n:

$$Q_\tau(\theta) = ||F\theta - y||^2 + \frac{1}{2\sigma}||\theta||^2 \to \min_\theta,$$

where $\tau = 1/\sigma$ is regularization penalty.

It can be simply added to OLS solution:

$$\theta_\tau^* = \left(F^\top F + \tau I_n\right)^{-1} F^\tau y.$$

Solution for ridge regression

$$\theta_\tau^* = U\left(D^2 + \tau I_n\right)^{-1} D V^\top y = \sum_{j=1}^{n} \frac{\sqrt{\lambda_j}}{\lambda_j + \tau} u_j (v_j^\top y);$$

$$F\theta_\tau^* = \left(VDU^\top\right)\theta_\tau^* = V\mathrm{diag}\left(\frac{\lambda_j}{\lambda_j + \tau}\right) V^\top y =$$

$$= \sum_{j=1}^{n} \frac{\lambda_j}{\lambda_j + \tau} v_j (v_j^\top y);$$

$$||\theta^*||^2 = ||D^2\left(D^2 + \tau I_n\right)^{-1} D^{-1} V^\top y||^2 == \sum_{j=1}^{n} \frac{1}{\lambda_j + \tau} \left(v_j^\top y\right)^2.$$

Tibshirani lasso

Assumption: values of vector θ has Laplacian distribution:

$$\begin{cases} Q_\tau(\theta) = ||F\theta - y||^2 \to \min\limits_{\theta}; \\ \sum\limits_{i=1}^{n} |\theta_i| \le \kappa. \end{cases}$$

LASSO (least absolute shrinkage and selection operator). Will lead to feature selection.

LASSO regression

The resulting optimization problem

$$Q_\tau(\theta) = ||F\theta - y||^2 + \tau\|\theta\|_1 \to \min_\theta,$$

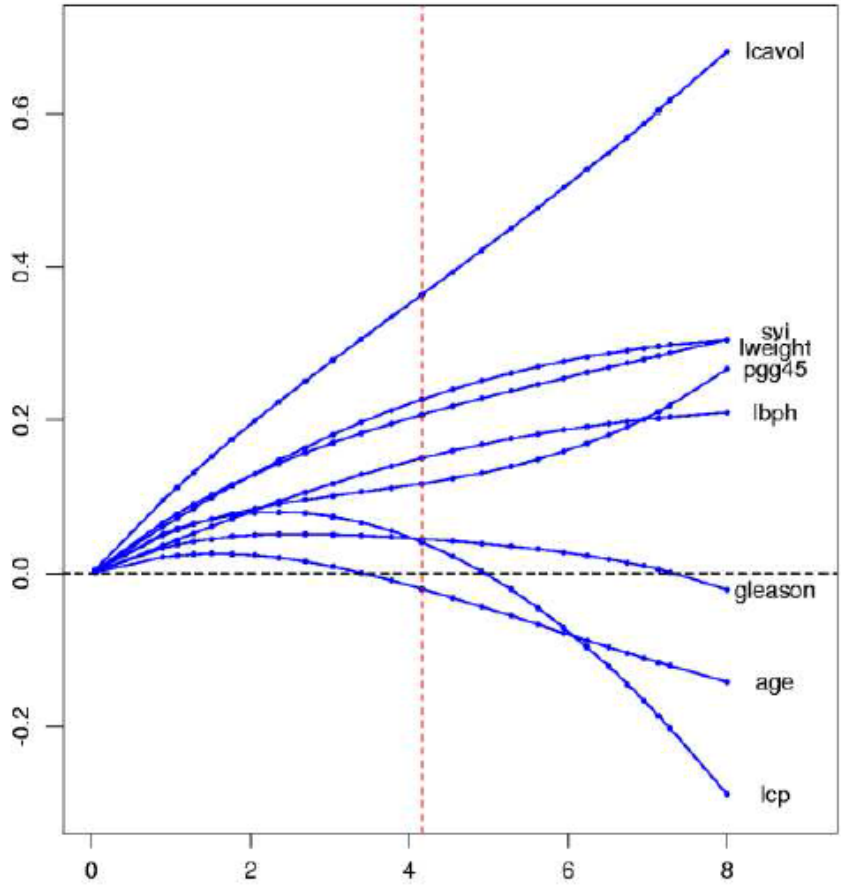
where $\|\theta\|_1$ is l_1-norm:$\|\theta\|_1 = \sum|\theta_i|$.

No nice analytical solution exist.

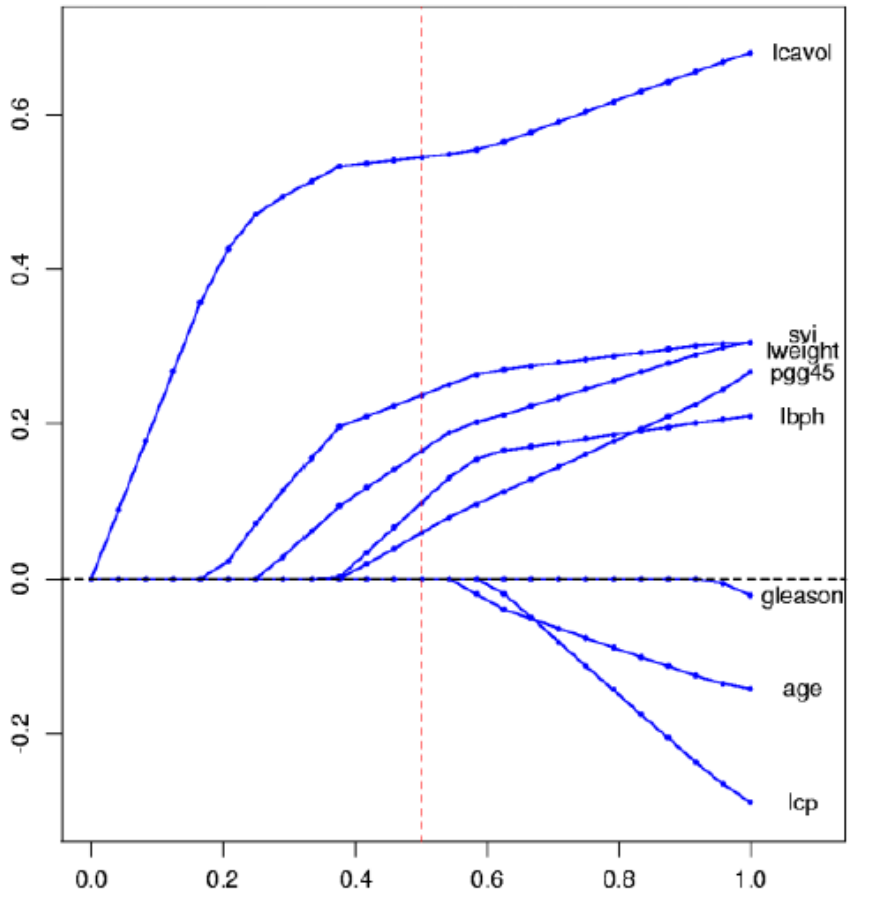
However, a nice computational solution exist.

Comparison

Ridge regression



Lasso



Regularization for gradient descent

Regularization is simply adopted to any gradient descent:

$$\nabla Q_\tau(w) = \nabla Q(w) + \tau w,$$
$$w^{[k+1]} = w^{[k]}(1 - \mu\tau) - \mu\nabla Q(w).$$

Regularization discussion (1/2)

- l_1-norm and l_2-norm regularizers are the most popular
- **ElasicNet**, which is sum of the previous two is also popular
- Many other may be used with respect to initial assumptions
- Some techniques are de-facto regularization or can be interpreted as regularization

Regularization discussion (2/2)

- One of two general approaches to fight overfitting
- Required to solve ill-stated problems
- Regularization penalties can be simply added to represent properties you expect from model

- Regularization coefficient should be tuned
- Not always clean, how to choose regularization