# Methods of Model Selection and Dimensionality Reduction

Vadim STRIJOV

Computing Center of the
Russian Academy of Sciences

Ankara, October 06, 2009
Institute of Applied Mathematics, METU

# Dimensionality reduction and index construction problem

- There is a set of objects, i.e. power plants:
    - Beckjord
    - East Bend
    - Miami Fort
    - Zimmer
- The **index** is a measure of an object's quality. It is a scalar, corresponded to an object.
- Expert estimation of an object's quality could be an index, too.

# Examples

| **Index name** | **Objects** | **Features** | **Model** |
|---|---|---|---|
| TOEFL | Students | Tests | Sum of scores |
| Eurovision | Singers | Televotes, Jury votes | Linear (weighted sum) |
| S&P500, NASDAQ | Time ticks | Shares (prices, volumes) | Non-linear |
| Bank ratings | Banks | Requirements | By an expert commission |
| Kyoto-index | **Power plants** | **Greenhouse gases** | **Linear** |

There are lots of ways to construct indices. However, when algorithms are chosen and some results obtained, the following question arises:

- **How to show adequacy of the calculated indices?**

To answer the question analysts invite experts. The experts express their opinion and then the second question arises:

- **How to show that expert estimations are valid?**

# How to construct an index?

- Assign a comparison criterion.
- Gather a set of comparable objects.
- Gather features of the objects.
- Make a data table: objects/features, i.e.

| # | Plant Name | Plant Type | Total Net Generation | $CO_2$ emission | NOx emission | SOx emission | Population density |
|---|---|---|---|---|---|---|---|
| | | | 10^6 KWHours | Shorttons per month | Shorttons per month | Shorttons per month | Qty per sq.mile |
| 1 | **Beckjord** | Coal | 458505 | 191 | 16 | 45 | 23 |
| 3 | **East Bend** | Coal | 356124 | 147 | 16 | 43 | 34 |
| 4 | **Miami Fort** | Coal | 484590 | 204 | 6 | 23 | 45 |
| 5 | **Dark Creek** | Coal | 818435 | 329 | 5 | 64 | 34 |
| | | **Optimal value** | **max** | **min** | **min** | **min** | **min** |

The criterion could be: **Ecological footprint of a plant**

# Notations

$A=\{a_{ij}\}$ – $(n \times m)$ real matrix, **data set**,

$\mathbf{q} = [q_1, \ldots, q_m]^T$ – vector of **object indices**,

$\mathbf{w} = [w_1, \ldots, w_n]^T$ – vector of

**feature importance weights**,

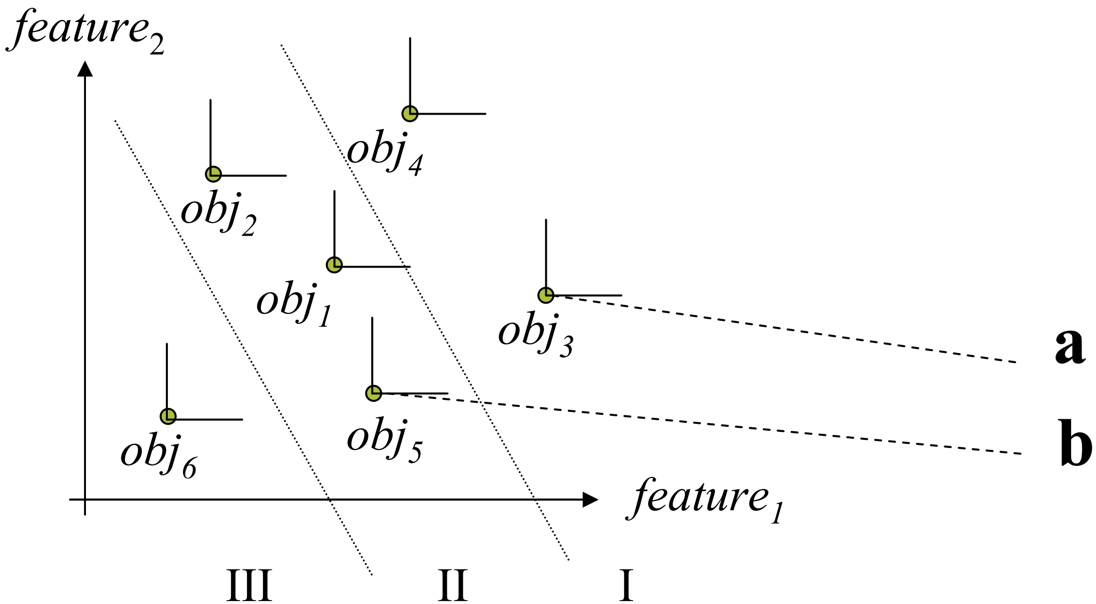
$\mathbf{q}_0$, $\mathbf{w}_0$ – **expert estimations of indices and weights**.

Usually, data prepared so that

1. the minimum of each feature equals 0, while the maximum equals 1;
2. the bigger value of each implies better quality of the index.

# The first method, Pareto slicing

An easiest method to obtain indices in ordinal scales is to find non-dominated objects at each slicing level.




The object **a** is non-dominated if there is no $\mathbf{b}_i$ such that $b_{ij} \geq a_i$ for all features $j$.

## Supervised way-1,

# the Weighted sum

$$\mathbf{q}_1 = A\,\mathbf{w}_0.$$

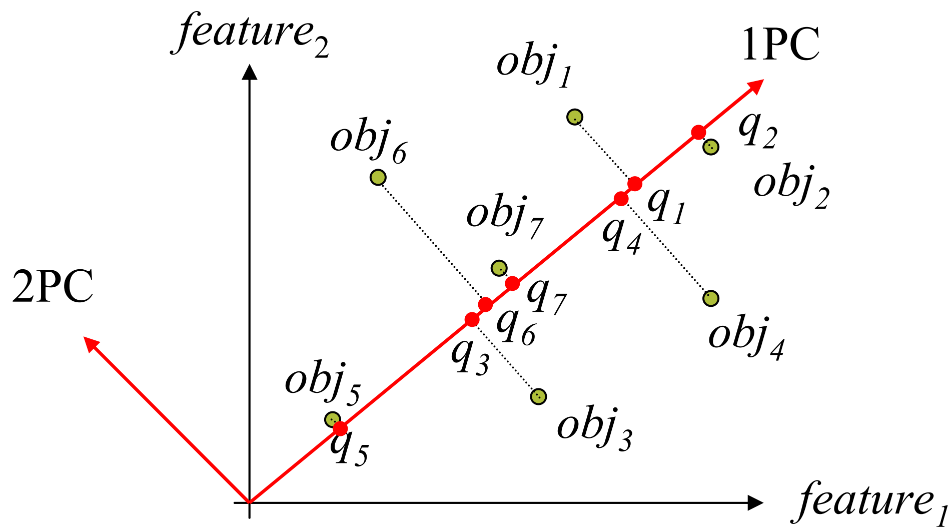
| | $w_1$ | $\dots$ | $w_n$ |
|---|---|---|---|
| $q_1$ | $a_{11}$ | $\dots$ | $a_{1n}$ |
| $\dots$ | $\dots$ | $\dots$ | $\dots$ |
| $q_m$ | $a_{m1}$ | $\dots$ | $a_{mn}$ |

Unsupervised way,

# Principal Components Analysis

$Q=AW$, where $W$—rotation matrix of the principal components.

$\mathbf{q}_{\mathrm{PCA}}=A\mathbf{w}_{1\mathrm{PC}}$, where $\mathbf{w}_{1\mathrm{PC}}$ is the 1st column vector of $W$.




PCA gives minimal mean square error between objects and their projections.

# useful tool for PCA

$$A = ULW^T$$

$$A^T A = WLU^T ULW^T$$

$$A^T AW = WL^2$$

## Supervised way-2,

## the Expert-Statistical Technique

$$\mathbf{w}_1 = \arg\min ||\mathbf{q}_0 - A\,\mathbf{w}||^2,$$

least squares, $\mathbf{w}_1 = (A^T A)^{-1} A^T \mathbf{q}_0.$

# The problem of specification

- **We have**

the data table *A*,

expert estimations $\mathbf{q}_0$, $\mathbf{w}_0$,

calculated weights and indices $\mathbf{q}_1$, $\mathbf{w}_1$.

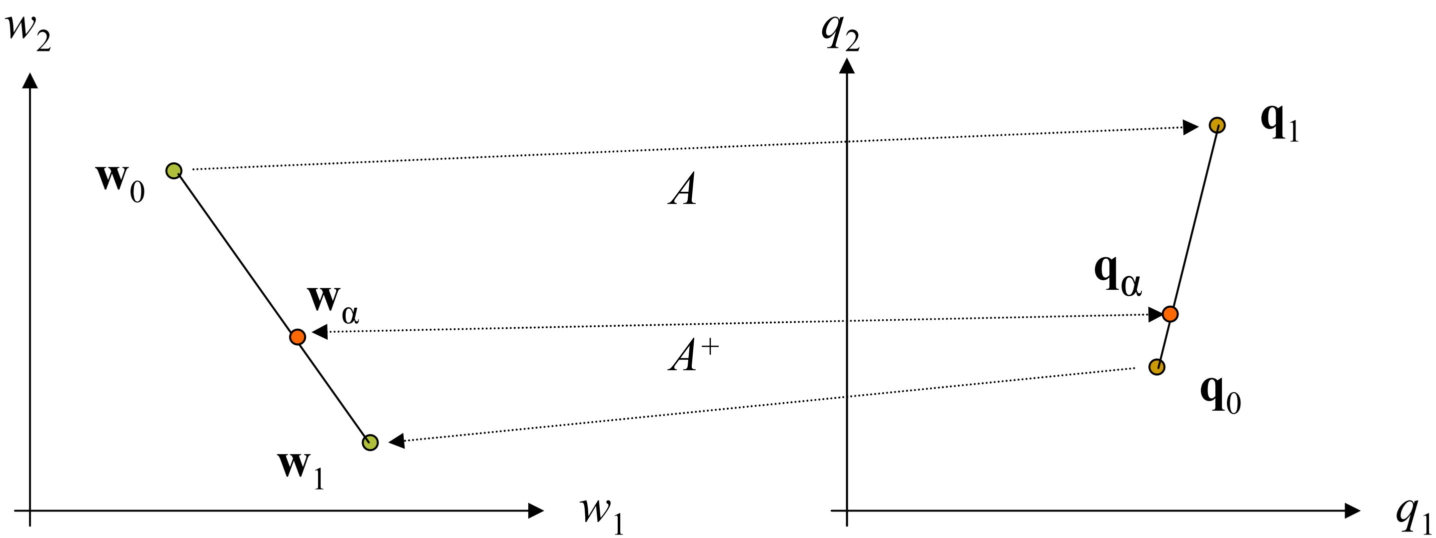
- **Contradiction**

Calculated indices are not the same as the expert estimations for the indices;

as well, calculated weights are not the same as the expert estimations of the weights:

**in general,**

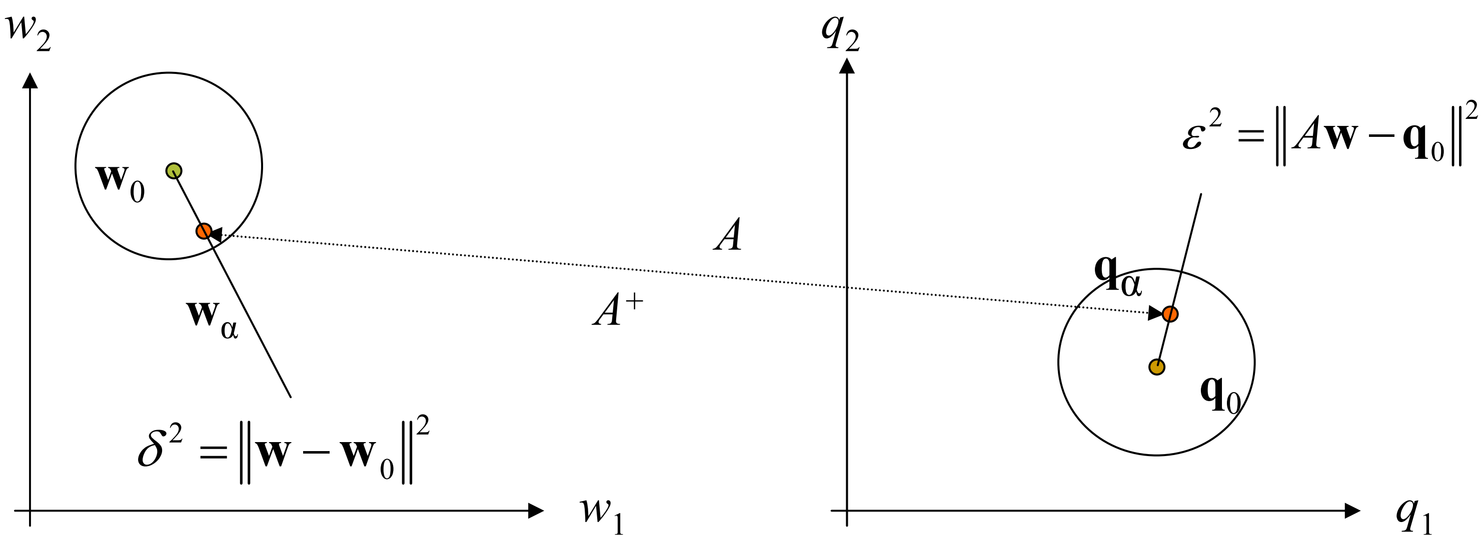
# Linear specification




$$\mathbf{w}_\alpha = \alpha A^+\mathbf{q}_0 + (\mathbf{1}-\alpha)\mathbf{w}_0, \qquad \mathbf{q}_\alpha = (1-\alpha)A\mathbf{w}_0 + \alpha\mathbf{q}_0.$$

Parameter $\alpha$ is in [0,1].
$\alpha = 0$, we trust expert estimations of the weights,
$\alpha = 1$, we trust expert estimations of the indices.

# Quadratic specification

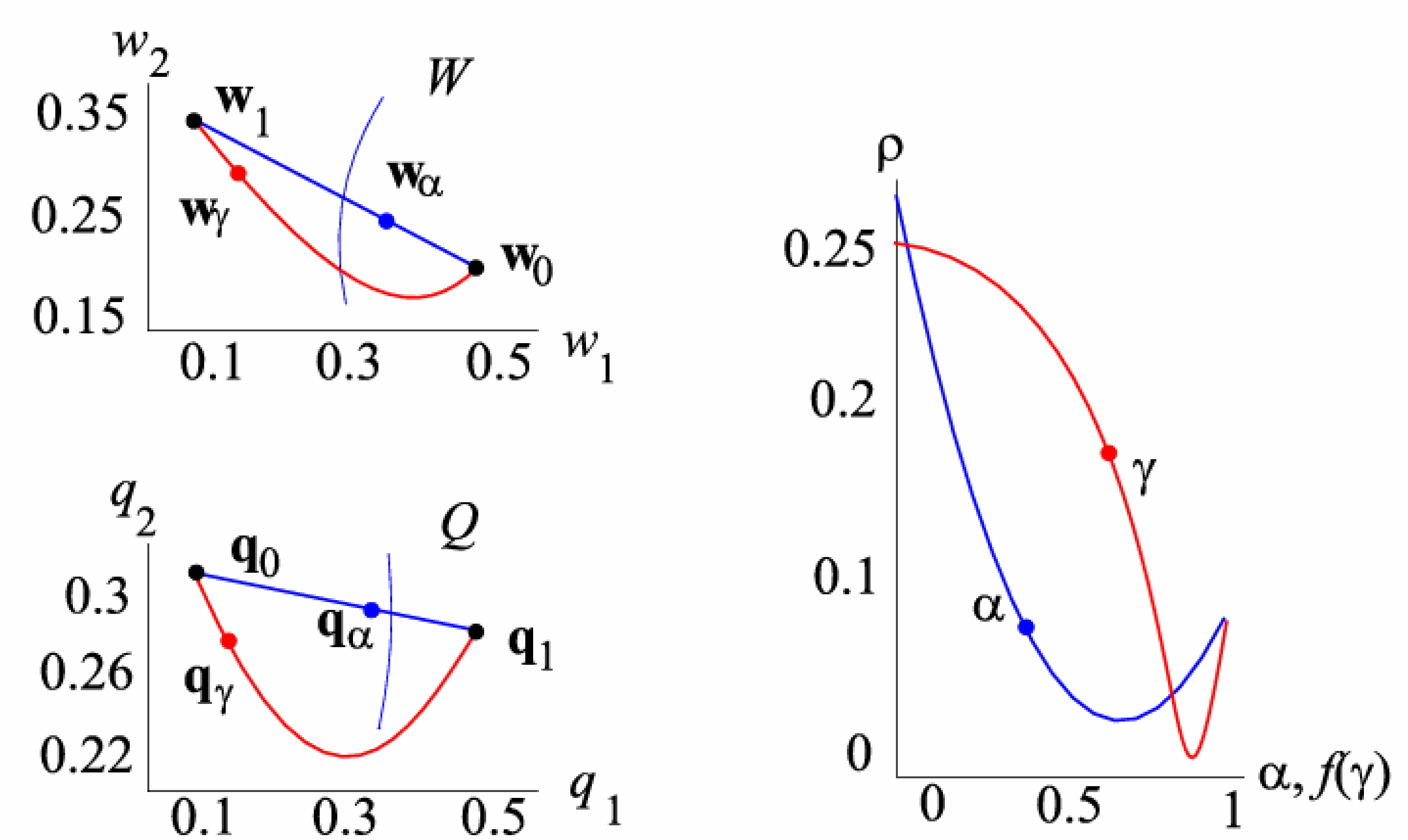



$$\mathbf{w}_\gamma = \arg\min_{\mathbf{w}\in W}(\varepsilon^2 - \gamma^2\delta^2), \quad \mathbf{w}_\gamma = (A^T A + \gamma^2 I)^{-1}(A^T\mathbf{q}_0 + \gamma^2\mathbf{w}_0).$$

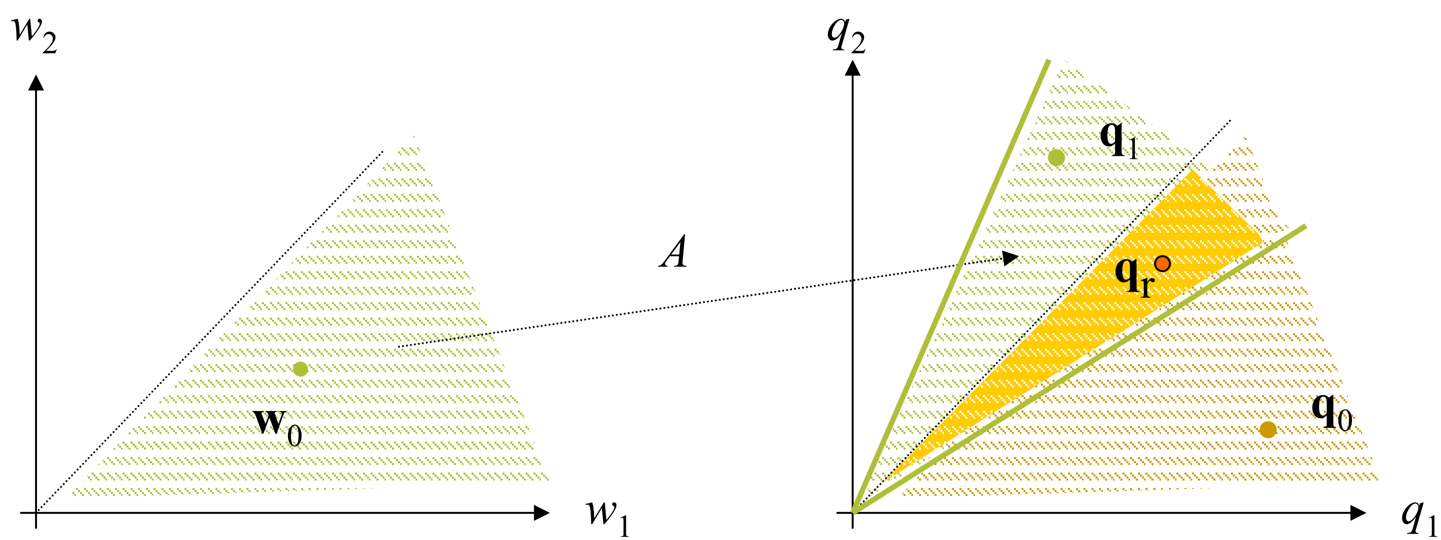
If parameter $\gamma^2$ is 0, then we trust expert estimations of the indices.

# Comparison of the methods,

what is the difference?



# Ordinal specification




$$\mathbf{w}_0 = [w_1 \geq w_2 \geq \ldots \geq w_n \geq 0]^T, \mathbf{q}_0 = [q_1 \geq q_2 \geq \ldots \geq q_m \geq 0]^T.$$

# Rank-scaled expert estimations

$$\mathbf{w}_0 = [w_1 \geq w_2 \geq \ldots \geq w_n \geq 0]^T, \mathbf{q}_0 = [q_1 \geq q_2 \geq \ldots \geq q_m \geq 0]^T.$$

$$Q_0 = \{\mathbf{q}_0 \mid J_m \mathbf{q}_0 \geq \mathbf{0}\},$$
$$W_0 = \{\mathbf{w}_0 \mid J_n \mathbf{w}_0 \geq \mathbf{0}\}.$$

$$J = \begin{pmatrix} 1 & -1 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & 1 \end{pmatrix}$$

# The cones intersection exists

$$\mathbf{q}_1 \in AW_0 \cap Q_0,$$

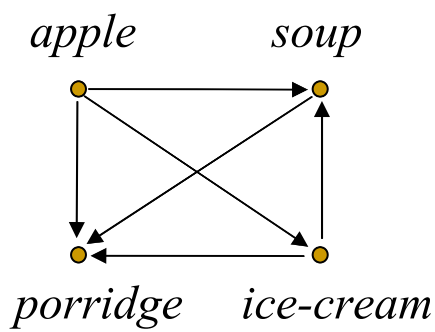
**or not, then specify**

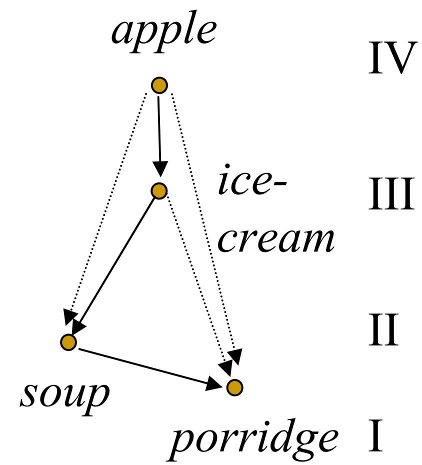
$$\mathbf{q}_\alpha = (1-\alpha)A\mathbf{w}' + \alpha\mathbf{q}', \quad \text{where}$$

$$\mathbf{w}', \mathbf{q}' = \arg \min_{\substack{\mathbf{w} \in W_0, \|\mathbf{w}\|^2 = 1 \\ \mathbf{q} \in Q_0, \|\mathbf{q}\|^2 = 1}} \|A\mathbf{w} - \mathbf{q}\|^2.$$

# Pair-wise comparison

| | *a* | *s* | *p* | *i-c* |
|---|---|---|---|---|
| *apple* | • | + | + | + |
| *soup* | | • | + | – |
| *porridge* | | | • | – |
| *ice-cream* | | | | • |




If an object in a row is better than the other one in a column then put "+", otherwise "-".

Make a graph, *row* + *column* means *row* $\bullet\!\longrightarrow\!\bullet$ *column.*

Find the top and remove extra nodes.

## The results of the specification are

- adequate indices,
- reasoned expert estimations.

We know why our expert valued each object
and what contribution each feature makes to the index.

## Model selection for (generalized) linear models

**Let there be given**

1. Sample set:
$\{(\mathbf{x}_i, y_i) | i = 1, \ldots, \ell\}$, where $\mathbf{x}_i \in \mathbb{R}^P, y_i \in \mathbb{R}^1$, $P = |N|$

- and $N \subset \mathbb{N}$.

s

2. Linear model:

$$y = f(\mathbf{w}, \mathbf{x}) + \varepsilon,$$
$$y = \langle \mathbf{w}, \mathbf{x} \rangle + \varepsilon.$$

3. Data generation hypothesis:
distribution of the random variable $\varepsilon_i$ is in the exponential family.
4. Target function:
minimum of the residual vector norm

$$SSE = \sum^{\ell} (\langle \mathbf{w}, \mathbf{x}_i \rangle - y_i)^2 \to \min .$$

## One must to

find a subset $\mathcal{A} \subset N$ of the indices $\hat{\mathbf{x}} = \{x_i^j | j \in \mathcal{A}\}$, such that the model $f(\mathbf{w}, \hat{\mathbf{x}})$ brings the optimum to the given criterion.

For example to the Colin Mallows' $C_P$:

$$C_P = \frac{SSE_P}{RMS} - \ell + 2P,$$

where

$$RMS = \frac{1}{\ell}\sum_{i=1}^{\ell}(y_i - f(\mathbf{w}, \mathbf{x}_i))^2.$$

Or to another criterion from the following list.

## Criterions for model selection

1. Information criterions
   - Akaike Information Criterion, $\mathrm{AIC} = 2P - 2\ln(S)$
   - Bayesian Information Criterion, $\mathrm{BIC} = P\ln(\ell) - 2\ln(S)$
2. Cross-validation
   - Retrospective Forecasting
   - Leave One Out
   - Random Split, etc.
3. Model Comparison
   - Bayesian Comparison
   - Minimum Description Length

## Superposition construction

Let there be given

- $\Xi = \{\xi^u\}_{u=1}^U$ — set of measured (nongenerated) independent variables,
- $G = \mathrm{id} \cup \{g_v\}_{v=2}^V$ — finite set of primitive functions.

Consider Cartesian product $G \times \Xi$. An element $(g_v, \xi^u)$ corresponds to the superposition $g_v(\xi^u)$ and defined by indices $v, u$.
Denote $s_\iota = g_v(\xi^u)$, where the index $\iota = (v-1)U + u$.

Consider $S \times S \times \ldots \times S$ — Cartesian product $\mathcal{N}$ of the sets $S = \{s_\iota\}$. Each element of $\mathcal{N}$ bijectively corresponds to the superposition $a_i = s_\iota^1 \circ s_\iota^2 \circ \ldots \circ s_\iota^{\mathcal{N}}$.

## Kolmogorov-Gabor polynomial

The basic model of the feature generation is

$$y = w_0 + \sum_{i=1}^{UV} w_i a_i + \sum_{i=1}^{UV} \sum_{j=1}^{UV} w_{ij} a_i a_j + \cdots + \sum_{i=1}^{UV} \ldots \sum_{z=1}^{UV} w_{i\ldots z} a_i \ldots a_z,$$

where the coefficients

$$\mathbf{w} = (w_0, w_i, w_{ij}, \ldots, w_{i\ldots z})_{i,j,\ldots,z=1,\ldots,UV}.$$

Represent this series as

$$y = \sum_{j \in N} w_j x^j.$$

The variables $\{x^j\}$ bijectively correspond to monomials of the polynomial.

## The model selection algorithms

Exhaustive search and modifications

1. Exhaustive search of $2^P$ models
2. Method of group data handling, $K \cdot C_P^2$ models
3. Genetic algorithms
4. Add (append a feature), $P(P-1)/2$ models
5. Del (eliminate a feature)
6. Add-del or stepwise regression, $\sim P^2$ models

Parameter space analysis

1. Least angle regression (LARS), Lasso
2. Optimal brain surgery

## Exhaustive search algorithm

The basic linear model includes all independent variables

$$y = w_0 + \alpha_1 w_1 x_1 + \alpha_2 w_2 x_2 + \ldots + \alpha_R w_P x_P.$$

The hyperparameter $\alpha \in \{0, 1\}$ is included for the model. The exhaustive search

$$\begin{array}{cccc} \alpha_1 & \alpha_2 & \ldots & \alpha_P \\ \hline 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 1 & 1 & \ldots & 1 \end{array}.$$

## Add (append a feature)

**Step 0.**
The active set $\mathcal{A}_0 = \emptyset$, and $N$ is the set if feature indices, $P = |N|$.
**Step** $k = 1, \dots, P$**.**
Select the next best feature index

$$\hat{j} = \arg \min_{j \in P \setminus \mathcal{A}_k} \min_{\mathbf{w} \in \mathbb{W}_k} \|(X_{\mathcal{A}_k} \vdots \mathbf{x}_j)\mathbf{w} - \mathbf{y}\|_2^2,$$

then

$$\mathcal{A}_{k+1} = \mathcal{A}_k \cup \hat{j}.$$

## Assume the following

The column vectors

$$\mathbf{x}^j = \{x_i^j | i \in 1, \ldots, \ell\} \quad \text{and} \quad \mathbf{y} = \{y_i | i \in 1, \ldots, \ell\}.$$

The model

$$\mathbf{y} = w_1\mathbf{x}^j + \ldots + w_P\mathbf{x}^P + \varepsilon,$$

in the other words,

$$\mathbf{y} = X\mathbf{w} + \varepsilon.$$

Assume for all $j \in N$

$$\|\mathbf{x}^j\|_1 = 0, \quad \|\mathbf{x}^j\|_2 = 1 \quad \text{and} \quad \|\mathbf{y}\|_1 = 0, \quad \|\mathbf{y}\|_2 = 1.$$

For all $j, k \in N$, $j \neq k$ the vectors $\mathbf{x}^j, \mathbf{x}^k$ are linear independent.
Then the vector of correlation coefficients

$$\mathbf{c} = X^T\mathbf{y}.$$

## Fast orthogonal search

**Step** 0.
The residuals $\varepsilon_0 = \mathbf{0}$, the active set $\mathcal{A}_0 = \emptyset$.

**Step** $k = 1, \dots, P$**.**

$$\mathcal{A}_k = \mathcal{A}_{k-1} \cup \hat{j},$$

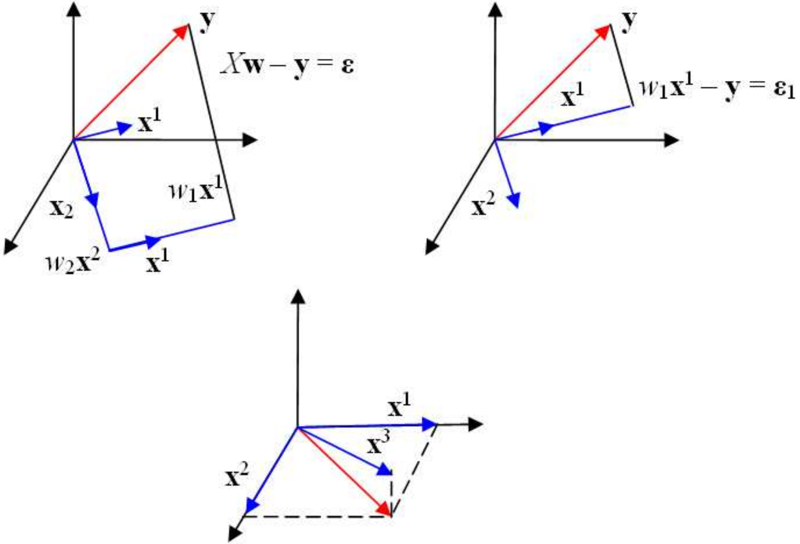
where $\hat{j}$ — feature, which has maximum correlation with $\varepsilon_k$:

$$\hat{j} = \arg \max_{j \in \{N \setminus \mathcal{A}_k\}} \frac{\langle \mathbf{w}, \mathbf{x}^j \rangle}{\|\mathbf{x}\| \|\varepsilon_k\|},$$

and

$$\varepsilon_k = X_{\mathcal{A}} \mathbf{w}_{\mathcal{A}} - \varepsilon_{k-1}.$$

## Fast orthogonal search



## Least angle regression, LARS

Denote $\boldsymbol{\mu} = X\mathbf{w}$.

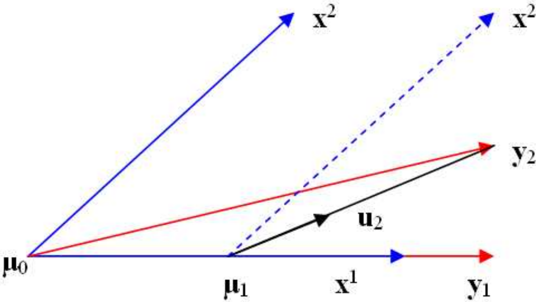
Step 0.
$\boldsymbol{\mu}_0 = \mathbf{0}$, residual vector $\varepsilon_0 = \mathbf{y} - \boldsymbol{\mu}_0$.

Step 1.
Let $\mathbf{y}$ has greater correlation with $\mathbf{x}^1$ than with $\mathbf{x}^2$. Then the new value of $\boldsymbol{\mu}_1 = \boldsymbol{\mu}_0 + w_1\mathbf{x}^1$, where $w_1$ is chosen so, that the vector $\mathbf{y}_2 - \boldsymbol{\mu}$ — is a bisector for the vectors $\mathbf{x}^1, \mathbf{x}^2$.

Step 2.
For the unit bisector $\mathbf{u}_2$ calculate $w_2$:

$$\boldsymbol{\mu}_2 = \boldsymbol{\mu}_1 + w_2\mathbf{u}_2 = \mathbf{y}_2 \quad \text{for P=2.}$$

# Least angle regression, LARS



## Lasso

Minimize the error

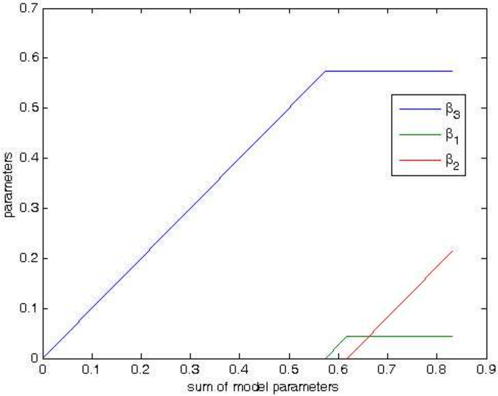
$$\|X\mathbf{w} - \mathbf{y}\|_2^2 \to \min,$$

subject to

$$\sum_{j \in N} \|w_j\|_1 \leqslant T.$$

**Theorem** (Efron et al., 2004).
Assuming the «one at time» condition, the LARS algorithm yields all Lasso solutions.

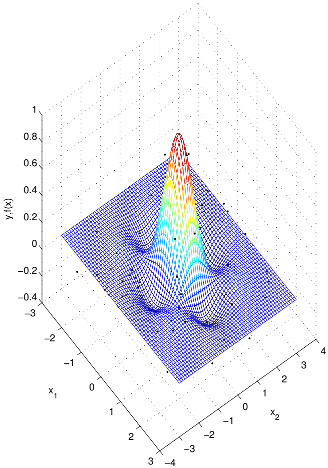
# Lasso and LARS

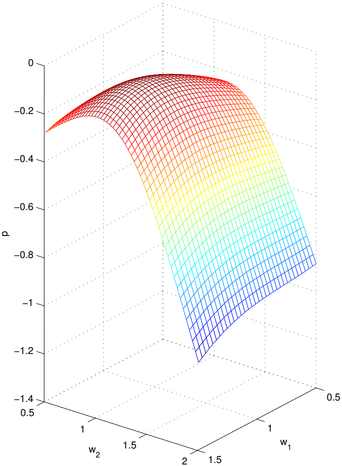


## Optimal brain surgery

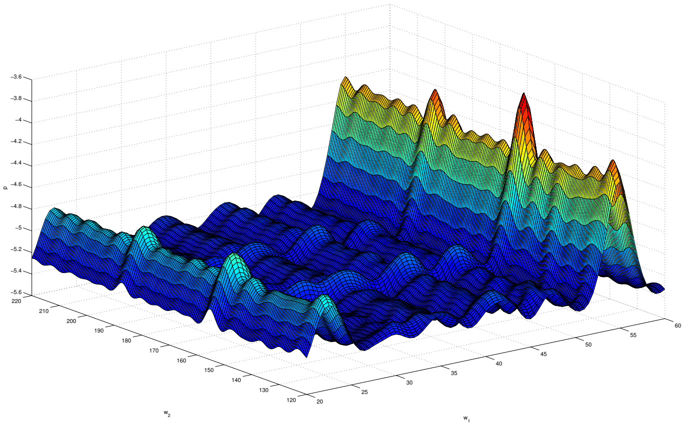
- Approximate $SSE = S(\mathbf{w})$:
  $S(\mathbf{w} + \Delta\mathbf{w}) = S(\mathbf{w}) + \mathbf{g}^T(\mathbf{w})\Delta\mathbf{w} + \frac{1}{2}\Delta\mathbf{w}^T H \Delta\mathbf{w} + o(\|\mathbf{w}\|^3)$.
- Elimination a feature is equivalent to $\mathbf{e}_i^T\Delta\mathbf{w} + w_i = 0$.
- Minimize the quadratic form $\Delta\mathbf{w}^T H \Delta\mathbf{w}$ subject to $\mathbf{e}_i^T + w_i = 0$, for all $i$.
- The index of the eliminated feature is $i = \arg\min_i(\min_{\Delta\mathbf{w}}(\Delta\mathbf{w}^T H \Delta\mathbf{w} | \mathbf{e}_i^T + w_i = 0))$.
- Introduce Lagrange function $S = \Delta\mathbf{w}^T H \Delta\mathbf{w} - \lambda(\mathbf{e}_i^T + w_i)$.
- For all $i$ $\Delta\mathbf{w} = -\frac{w_i}{[H^{-1}]_{ii}} H^{-1}\mathbf{e}_i$.
- The salience of the target function is $L_i = \frac{w_i^2}{2[H^{-1}]_{ii}}$.

# Optimal brain surgery



# Optimal brain surgery



*Ventia non sunt multiplicanda praeter necessitatem*

William of Ockham
1285-1349

**Occam's rasor:** entities (model elements) must not be multiplied beyond necessity