# A Self-Adapting System for Linear Solver Selection

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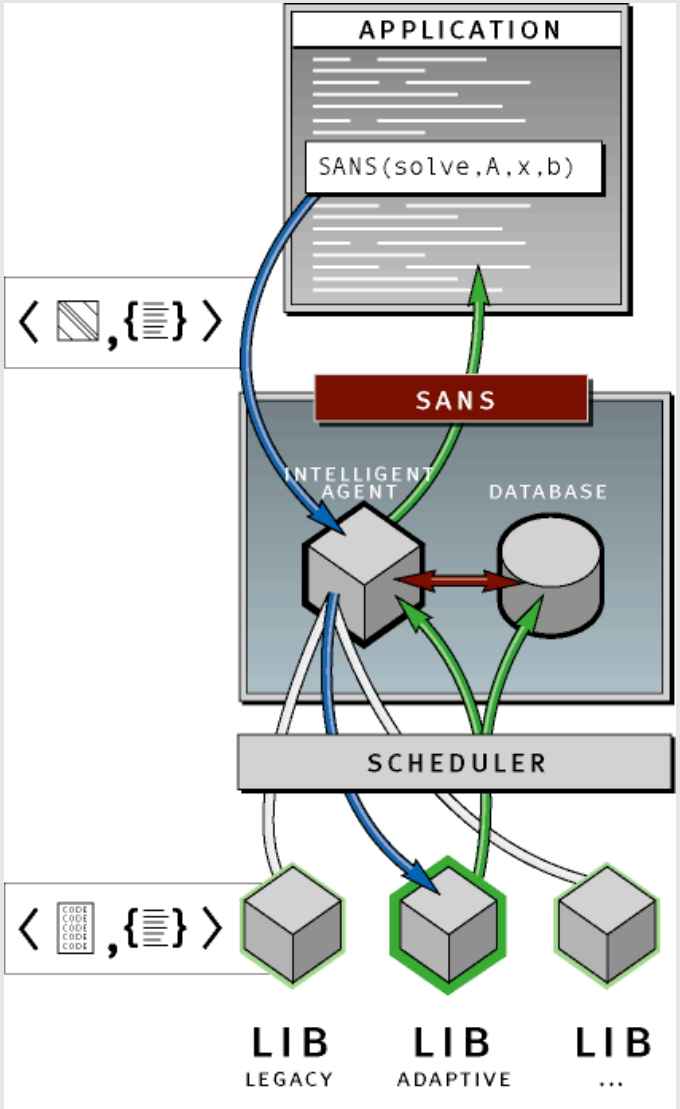
# Self-Adapting Numerical Software; problem statement

On several levels of a scientific problem-solving environment, decision are beyond the user's province.

- Kernel performance is not portable or persistent
- Scheduling of parallel jobs is extremely dynamic
- Solving scientific problems takes numerical knowledge outside the application field

# Proposed solution

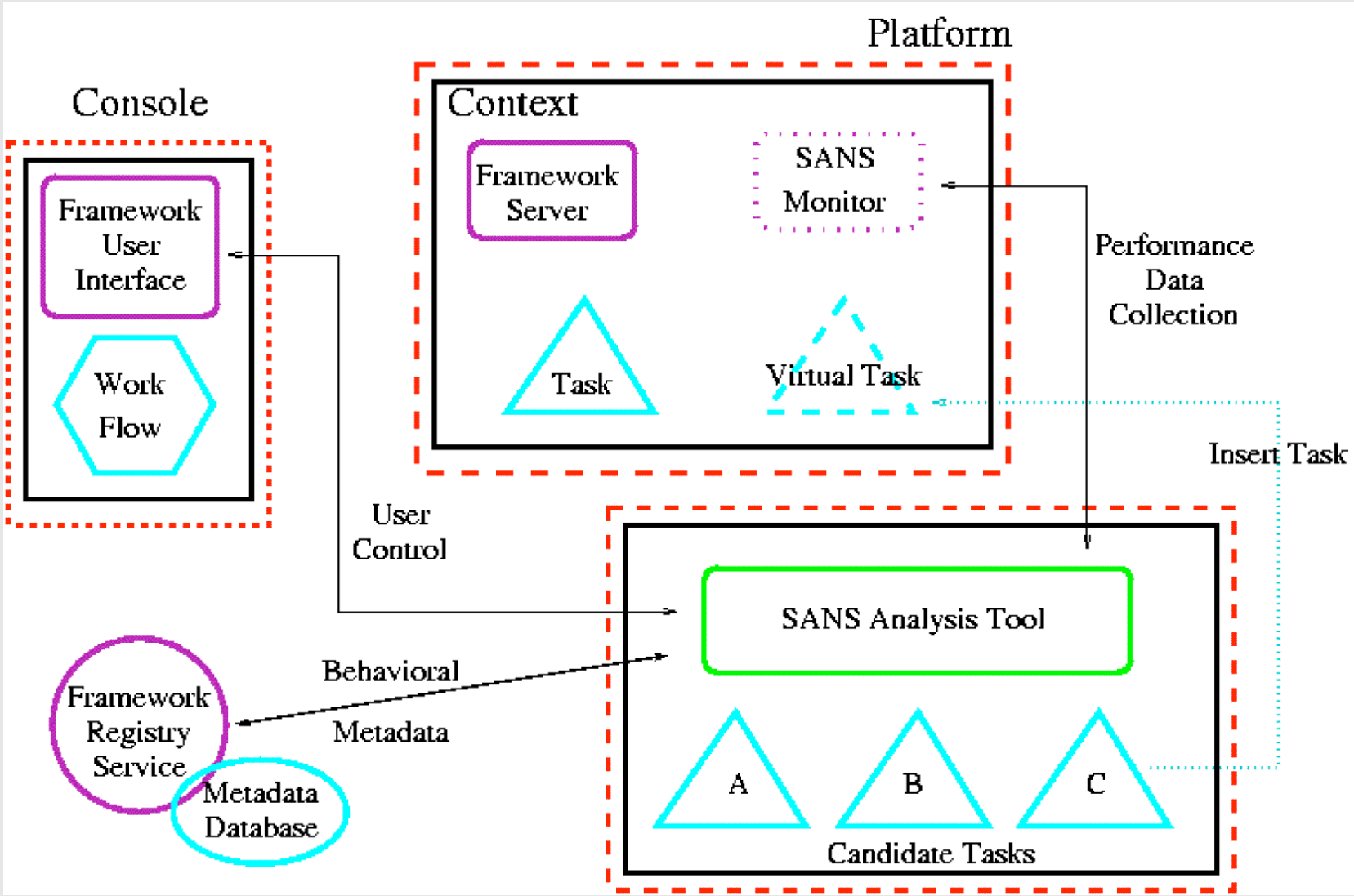
- Adaptive software: inspect user data and computational platform, find best algorithm
- Heuristic investigation: most questions can not be answered exactly; we settle for good enough
- Self-adapting software: remember results of production runs, learn over time




Three levels of adaptivity

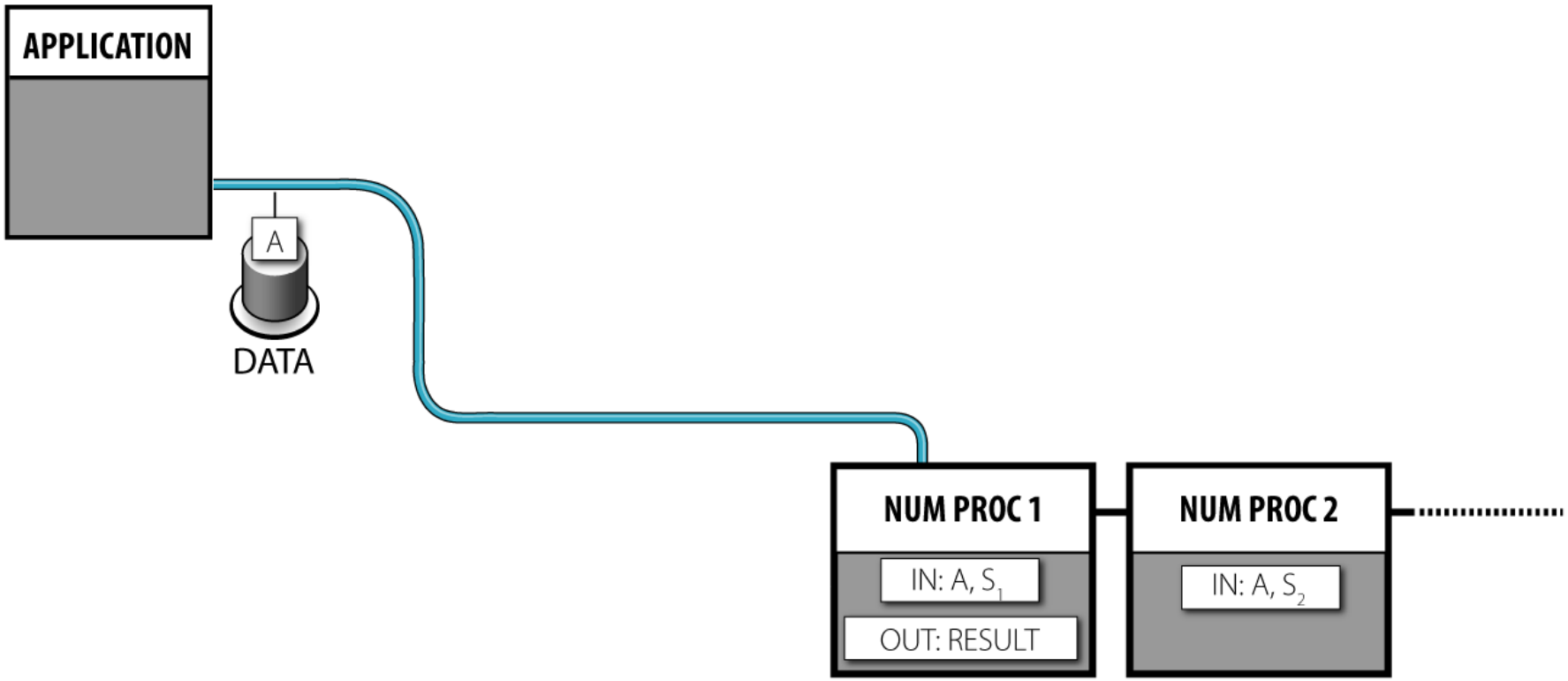
- Kernel level: Atlas and such; independent of user data, can be done in one-time installation
- Network level: Grads and such; modest interaction with user data, but no major influence
- Algorithm level: analysis dynamically, completely based on user data

# Component-based framework

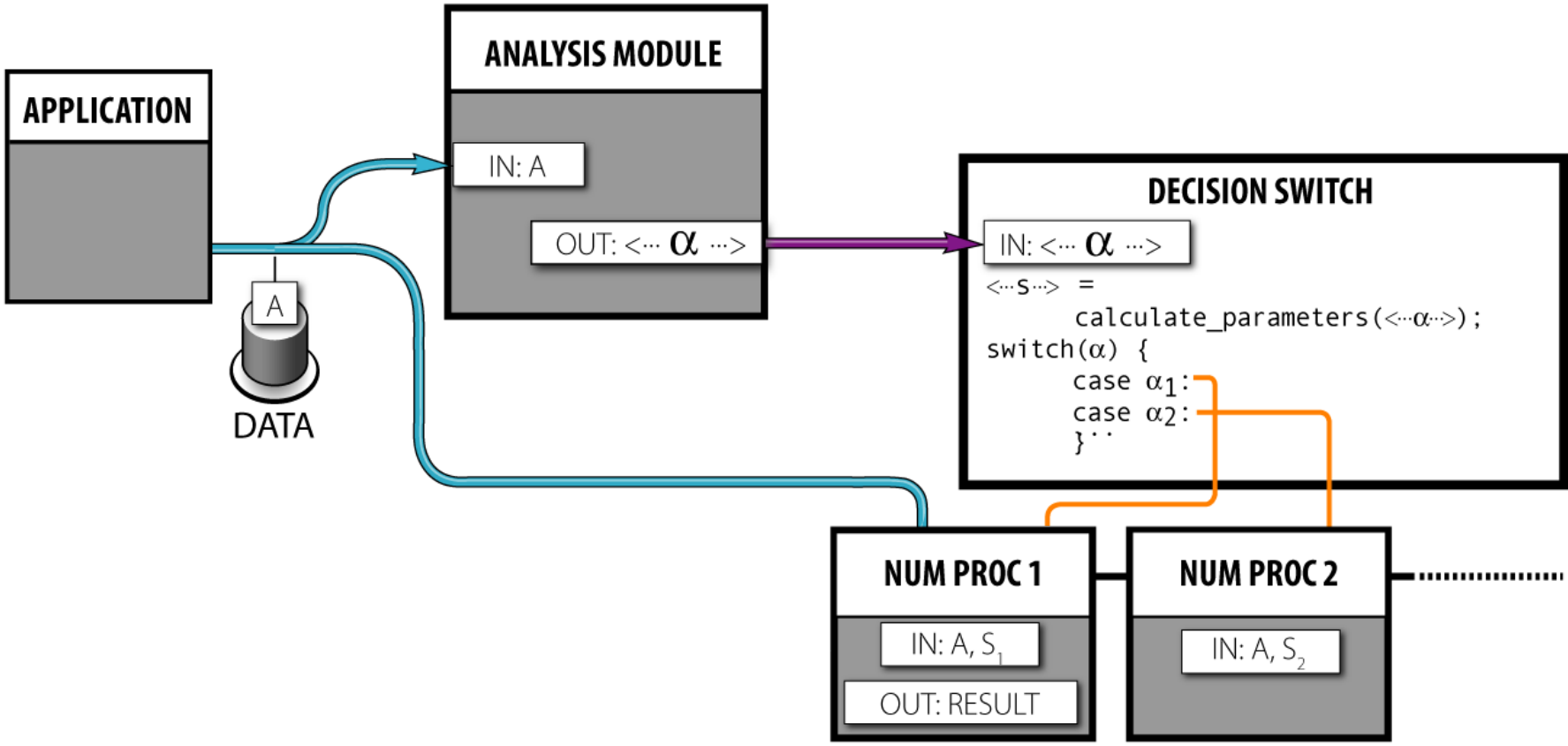


# Adaptive algorithm choice

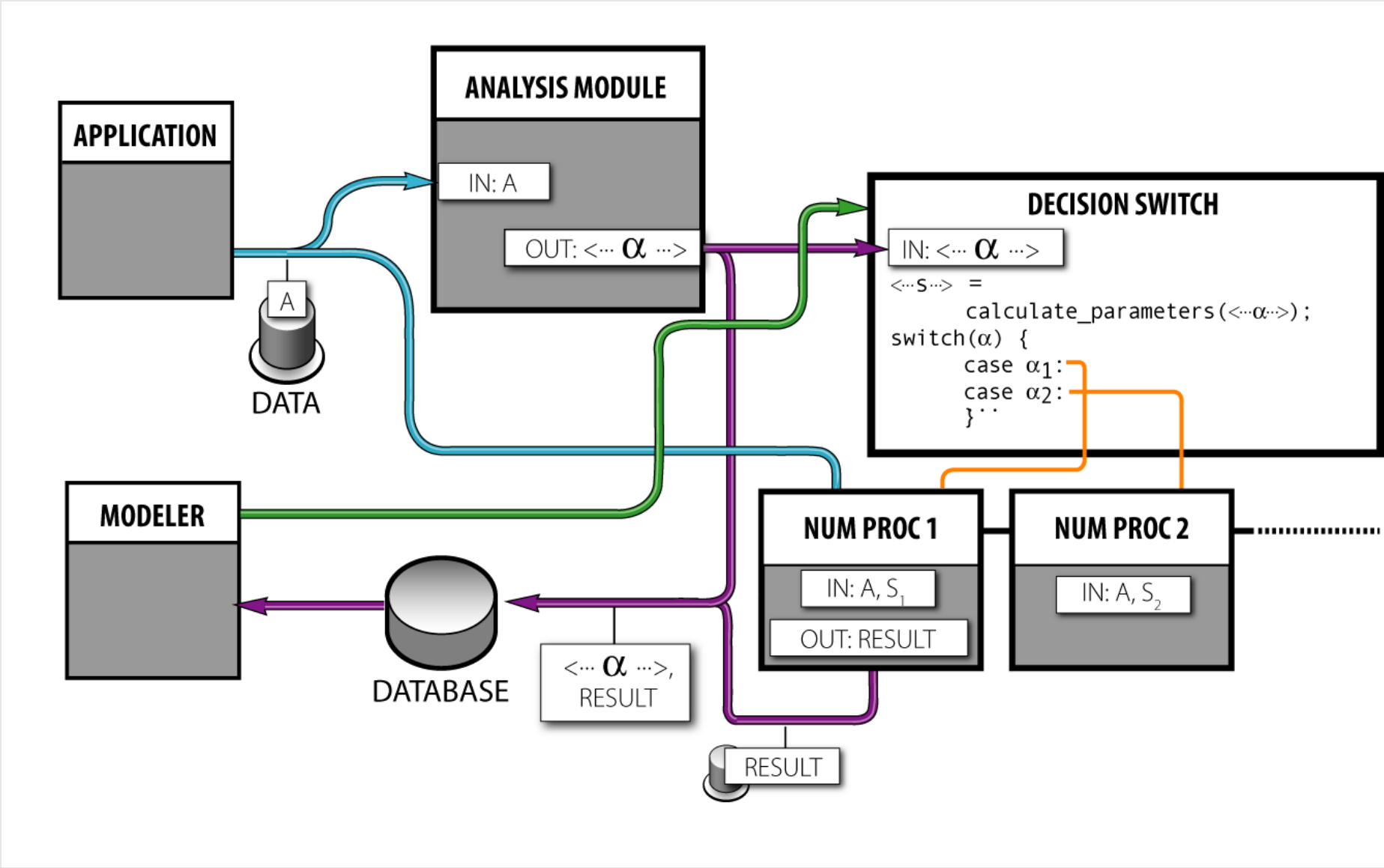
# Hand-coded decisions



# Use of analysis modules



# Self-adaptive system



# Abstract description of adaptive systems

# Numerical problems

$\mathbb{A}$: *the set of numerical problems in a class*

Dependent on the application area
linear systems:

```
struct Problem_ {
    LinearOperator A;
    Vector RHS,KnownSolution,InitialGuess;
    double desired_accuracy;
};
typedef struct Problem_* Problem;
```

# Results

$\mathbb{R} = \mathbb{S} \times \mathbb{T}$: *results, the space of solutions plus performance measurements*

```
struct Result_ {
    Vector ComputedSolution;
    PerformanceMeasurement performance;
}
struct PerformanceMeasurement_ {
    int success;
    double Tsetup,Tsolve;
    double *ConvergenceHistory;
    double BackwardError,ForwardError;
}
```

# Solution methods

$\mathbb{M} = \{\mathbb{A} \mapsto \mathbb{R}\}$: *the space of methods (potentially) solving the class of numerical problems*

```
Solver(Problem problem,Result *solution);
```

In the SALSA system, the solvers are the `KSP` objects of the Petsc library.

# Method selection

$T(A, M)$: time taken by method $M$ on problem $A$

Function $\Pi : \mathbb{A} \mapsto \mathbb{M}$

$$\Pi(A) = M \quad \equiv \quad \forall_{M' \in \mathbb{M}} : T(A, M) \leq T(A, M')$$

Often enough:

$$\Pi'(A) = M \quad \equiv \quad M \text{ is such that } T(A, M) < \infty$$

Defining $\Pi$ in terms of $\mathbb{A}$ impractical: need problem features

# Features, metadata

$\mathbb{F}$: *the space of features of the numerical problems*

Features (Numerical Metadata) is divided in categories and elements.

Example categories: structural, normlike, spectral

Often a single computational function for one category.

# Feature classes

| | |
|---|---|
| structure | Structural symmetry, bandwidth, sparsity, skyline |
| iprs | more structural properties |
| simple | various norms, including norm of symmetric/antisymmetric part |
| variance | diagonal average and variance |
| normality | various measure of departure from normality |
| spectrum | ellipse around FOV, condition, max/min singular values |
| $\Rightarrow$ | 75 features in all |

# The NMD library

# Metadata API

In SALSA: NMD library

```
NMDCreateObject(NMD_metadata *obj);
NMDCreateCategory(NMD_metadata,char *cat);
NMDCreateComponent
      (NMD_metadata,char *cat,char *cmp,NMDDataType t);
NMDSetValue(NMD_metadata,char *cat,char *cmp,void *val);
NMDGetValue(NMD_metadata,char *cat,char *cmp,
       NMDDataType *t,void *val,int *success);
```

# NMD capabilities

- Storage and retrieval
- Manipulation of whole categories
- Conversion to XML, display with XSL

# The AnaMod library

# Feature extraction

$\Phi : \mathbb{A} \mapsto \mathbb{F}$: *a function that extracts features of numerical problems*

```
ComputeQuantity(Problem problem,
  char *cat, char *cmp,ReturnValue *result,TruthValue *success);
```

Modular design:

```
DeclareModule(char *cat,char *cmp,ReturnType type,
    void(*module)(Problem,char*,char*,ReturnValue*,TruthValue*));
```

# Method selection, 2nd try

$\Pi : \mathbb{F} \mapsto \mathbb{M}$: *the function that picks the best solution method*

$\Pi(\bar{x}) = M$ if $\Phi(A) = \bar{x}$ and $M$ s.t. $\forall_{M' \in \mathbb{M}} : T(A, M) \leq T(A, M')$.

(what if $\Phi(A_1) = \Phi(A_2)$?)
Method picking:

$$\Pi \circ \Phi : \mathbb{A} \mapsto \mathbb{M}$$

*Intelligent Solver*:

$$Q = \lambda(A)\Pi(\Phi(A))(A)$$

Complication: methods are actually compound objects

# The SysPro library

# Preprocessors

$\mathbb{P} = \{\mathbb{A} \mapsto \mathbb{A}\}$: *the set of all mappings from problems into problems*

Example: scale or permute a linear system

$\mathbb{K} = \{\mathbb{A} \mapsto \mathbb{R}\}$: *the set of all solvers*

Example: iterative and direct methods

$$m \in \mathbb{M}\colon\ m = k \circ p_n \circ \cdots \circ p_1, \quad k \in \mathbb{K}, p_i \in \mathbb{P}_i$$

# Preprocessor classes

$$m \in \mathbb{M}\colon\ m = k \circ p_n \circ \cdots \circ p_1, \quad k \in \mathbb{K}, p_i \in \mathbb{P}_i$$

Each preprocessor belongs to a class:

$$\mathbb{P} = \mathbb{P}^1 \cup \cdots \mathbb{P}^n, \qquad p_i \in \mathbb{P}^i$$

For instance: left / right / symmetric scaling.

# Preprocessor implementation

$$\mathbb{P} = \{\mathbb{A} \mapsto \mathbb{A}\}$$

```
SystemPreprocessor(char *type,char *choice,
    Problem in,Problem *out);
```

Dynamic discovery:

```
DeclarePreprocessor(char *type,char *choice,
    void(*preprocessor)(Problem,Problem*),
    char *required_features,int nreq);
```

# Method selection, 3rd try

$\Pi_i : \mathbb{F} \mapsto \mathbb{P}_i$: *the selector function for preprocessor i*

$\Pi_k : \mathbb{F} \mapsto \mathbb{K}$: *the method selector*

Intelligent preprocessor application:

$$Q_i = \lambda(A)\Pi_i(\Phi(A))(A)$$

$\Rightarrow Q_i \in \mathbb{P}$.

# The ModBaR library

# Method suitability

Suitability functions:

| |
|---|
| $\mathbb{S} = \{\mathbb{F} \to [0,1]\}$: the space of suitability measurements of feature vectors |

"Conjugate gradient method: only for symmetric positive definite" (semantic specification of library routines)

| |
|---|
| $\mathbb{B}: \mathbb{M} \to \mathbb{S}$: the method suitability function |

then

$$\Pi(f) = \arg\max_{m} \mathbb{B}(m)(f).$$

# Classifier construction

$\mathbb{D}\colon \mathbb{F} \times \mathbb{M} \to \mathbb{T}$: *the database of features and performance results of solved problems*

Mark the best method among those tested:

$$\mathbb{D}'\colon \mathbb{F}\times\mathbb{M} \to \{0,1\} \quad \Leftrightarrow \quad \mathbb{D}'(f,m) = 1 \;\equiv\; m = \underset{m\colon (m,f)\in\mathbb{D}}{\arg\min}\; \mathbb{D}(f,m)$$

Describe problems solved best by each method:

$$\mathbb{B}'\colon \mathbb{M} \to P(\mathbb{F}) \quad \text{defined by} \quad f \in \mathbb{B}'(m) \Leftrightarrow \mathbb{D}'(f,m) = 1$$

Classifier construction

$$\mathbb{C}\colon P(\mathbb{F}) \to \mathbb{S}$$

Then $\mathbb{B} = \mathbb{C} \circ \mathbb{B}'$.

# Implementation of classifier construction

Requires functional language; implementation in C possible

# Declare suitability function

```
FeatureSet symmetry;
NewFeatureSet(&symmetry);
AddToFeatureSet
  (symmetry,"simple","symmetry-snorm",PETSC_NULL);
AddToFeatureSet
  (symmetry,"simple","symmetry-anorm",PETSC_NULL);
PreprocessorSetSuitabilityFunction
  (cur,(void*)symmetry,&onlyforsymmetricproblem);
```

# Use suitability function

```
void onlyforsymmetricproblem
    (NumericalProblem p,FeatureSet s,SuitabilityValue *val)
{
NewFeatureValues(&values);
InstantiateFeatureSet(p,s,values);
GetFeatureValue(values,0,&sn,&f1);
GetFeatureValue(values,1,&an,&f2);
if (f1 && f2 && an.r>1.e-12*sn.r) {
  *val = ....   /* problem too unsymmetric */
}
}
```

# The Salsa System

# Capabilities of Salsa

- Extraction of features
- Storage of features
- Testbed for iterative linear system solvers (direct, nonlinear)
- Statistical analysis
- Automatic heuristic building and application
- Application monitor, dynamic testing, heuristic tuning
- . . . under development. . .

# Solver capabilities

- Using Petsc:
- Iterative solvers and preconditioners
- Pre-processing of the system: scaling, distribution, approximation, Schur complement (not yet implemented)

# Machine Learning / Statistical analysis

# Statistical approach

- Method choice can be approached as a classification problem
  - Class $\equiv$ Method
  - Classifier $\equiv$ Way of picking method
- Fuentes: Bayesian decision theory
- Ramakrishnan and Kang: Reinforcement Learning
- Bhowmick/Freund/Keyes: Boosting, Decision trees
- Zhang: Support Vector Machines (not in Salsa)

# Bayesian decision making

# Bayesian decision theory

Picking a method becomes a classification problem:

> *Given problem features $\bar{x}$, for which method $\omega_i$ is the suitability $P(\omega_i|\bar{x})$ maximized.*

# Bayesian decision theory'

- Take large set of test problems $\bar{x}$, and test them with all methods
- Assign them to the class of the fastest method
- $\Rightarrow$ Method $\equiv$ Class $\equiv$ set of problems on which this method is the fastest
- Construct the probability density functions (see below)
- Method choice: for a problem with features $\bar{x}$, take class $i$ that maximizes $P(\omega_i|\bar{x})$

# Bayesian decision theory

- Bayes' theorem:

$$P(A|B) = \frac{P(B|A)P(B)}{P(A)}$$

(from $P(A \wedge B) = P(A|B)P(B) = P(B|A)P(A)$)

- Used as:
  let $x$ be a feature vector, $\omega_i$ a class

$$P(\omega_i|\bar{x}) = \frac{P(\bar{x}|\omega_i)P(\bar{x})}{P(\omega_i)}$$

'what is the chance $\omega_i$ is the best method for problem $\bar{x}$'

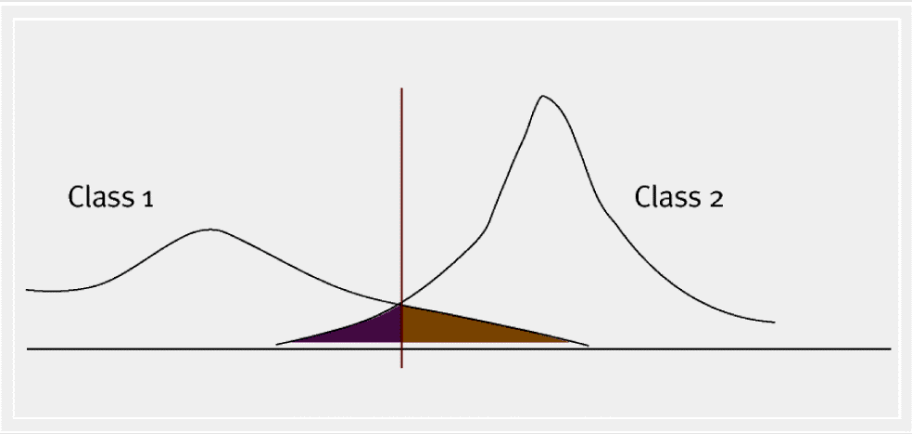
# Class-conditional probability

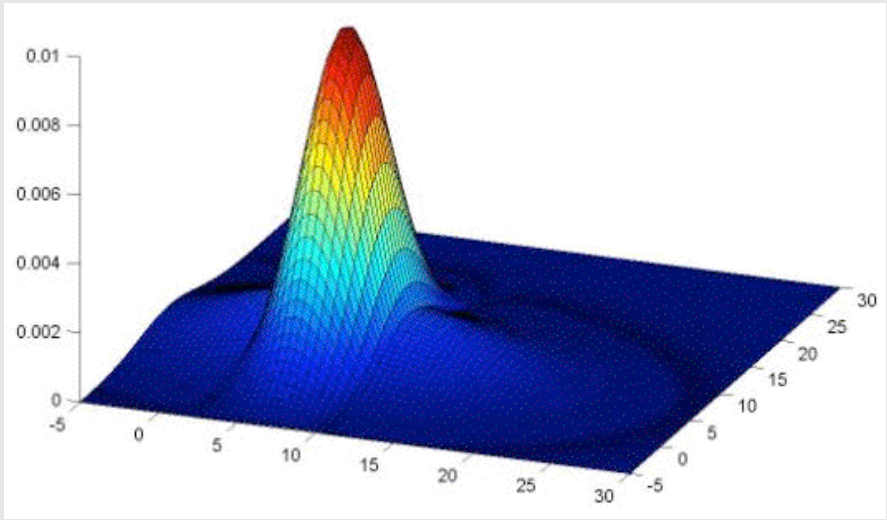
$$P(\omega_i|\bar{x}) = \frac{P(\bar{x}|\omega_i)P(\bar{x})}{P(\omega_i)}$$

- Most important quantity: 'class-conditional probability' $P(x|\omega_i)$
- Choice of 'probability density function'
- Assumption of Gaussian distribution:

$$P(\bar{x}, \bar{\mu}, \Sigma) = \frac{1}{(2\pi)^{d/2}|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(\bar{x}-\bar{\mu})^t\Sigma^{-1}(\bar{x}-\bar{\mu})\right\}.$$

where mean $\bar{\mu}$ and variance $\Sigma$ derived from data


Class 1
Class 2


0.01
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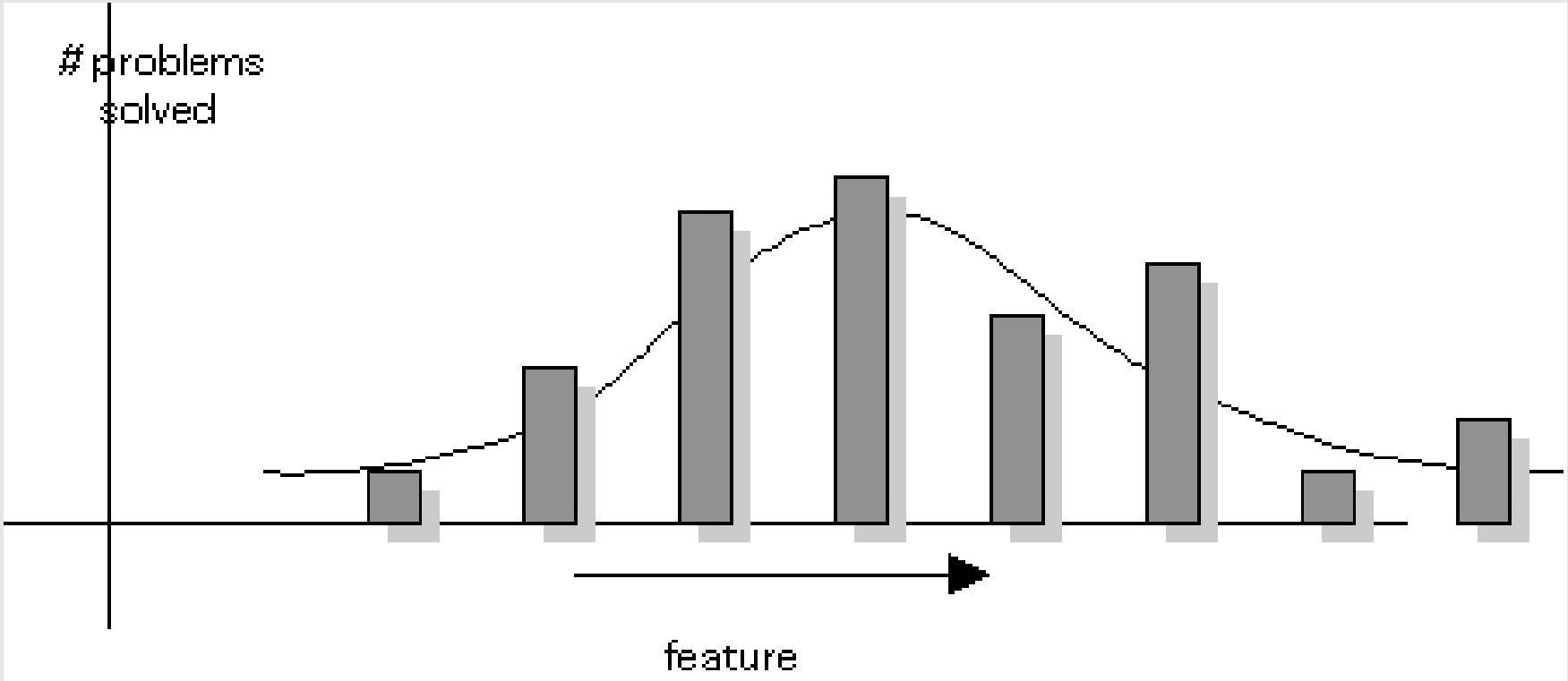
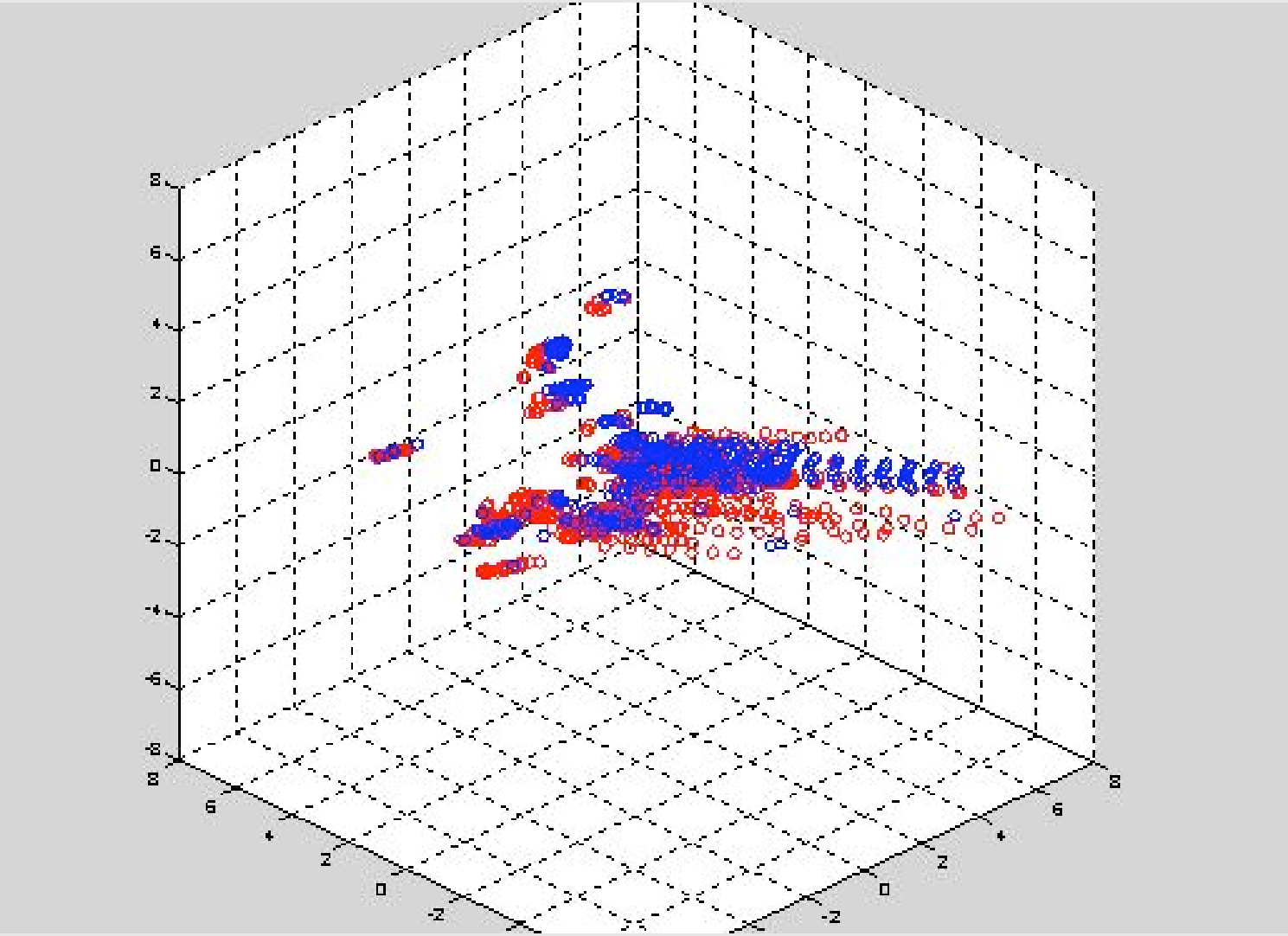
0.006
0.004
0.002
0
-5
0
5
10
15
20
25
30

# Gaussian assumption

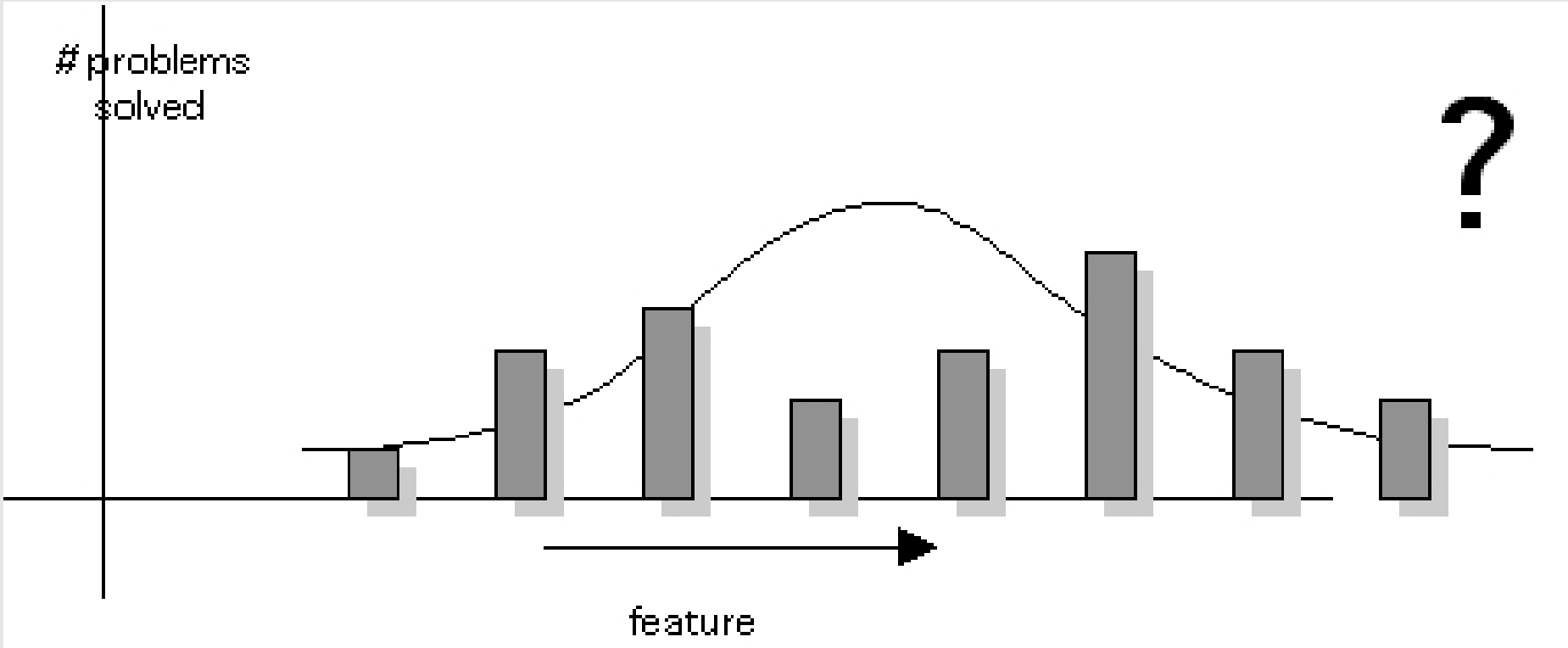


# Discriminant analysis

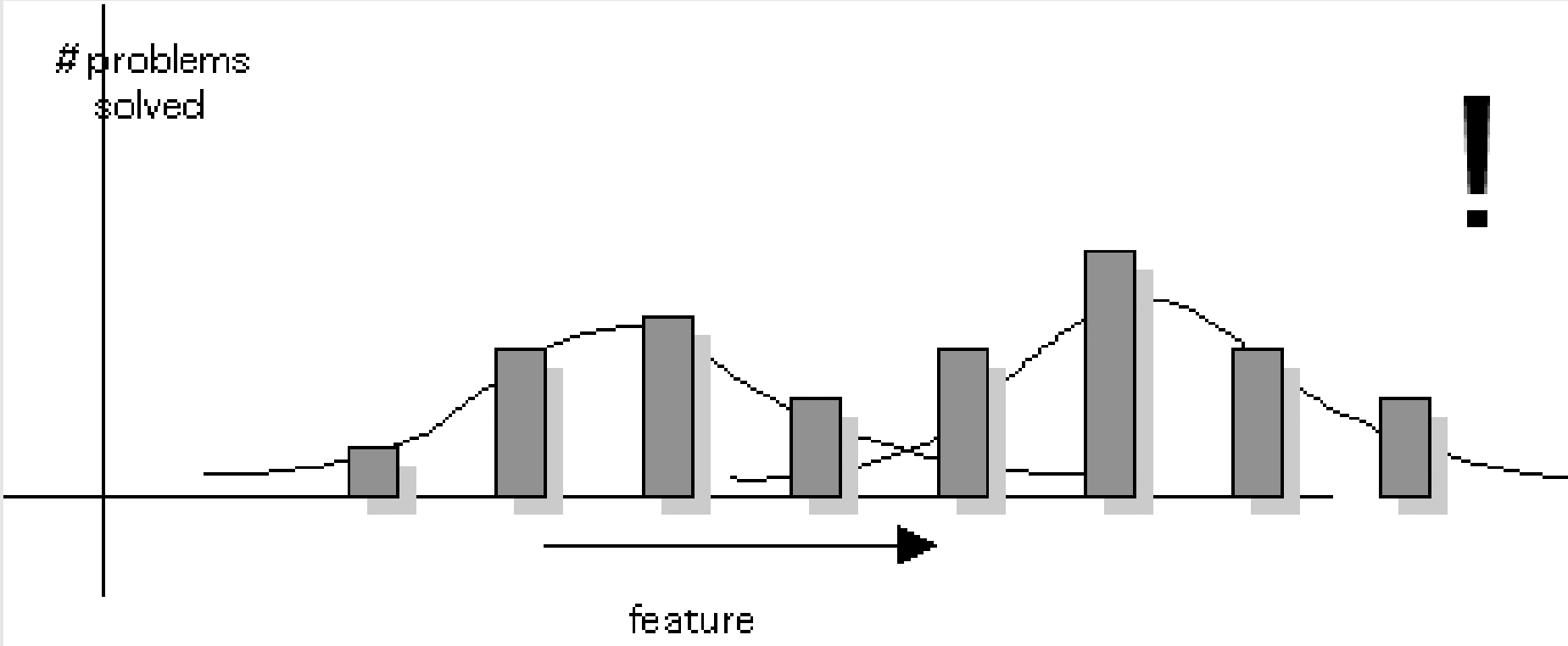
The assumption of a Gaussian distribution may not be justified:



# Kernel mixtures



# Kernel mixtures



# Test of Bayesian classification

# Outline of the test

- Apply principal component analysis (PCA) to features
- Use principal components to classify iterative methods:
  bcgs, gmres, tfqmr, direct
  maximum over all other options

# Relevant features

2 trace/norminf

7 symm_anorm/symm_snorm

10 row_variability

25 ellipse_ay/ax

28 kappa

29 positive_fraction

31 sigma_min / norm1

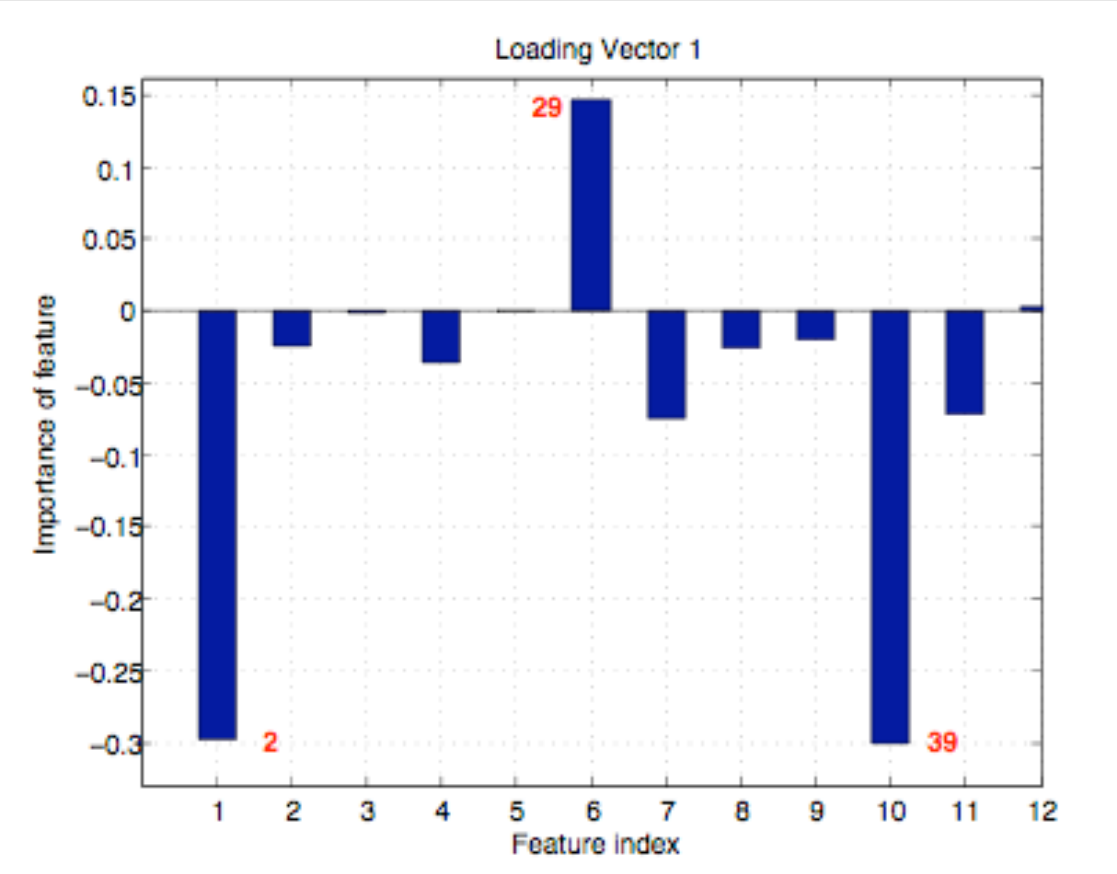
33 lambda_max_mag_im/norm1

34 lambda_min_mag_re/ lambda_max_mag_re

39 commutator_normF/ normF$^2$

40 ruhe75_bound

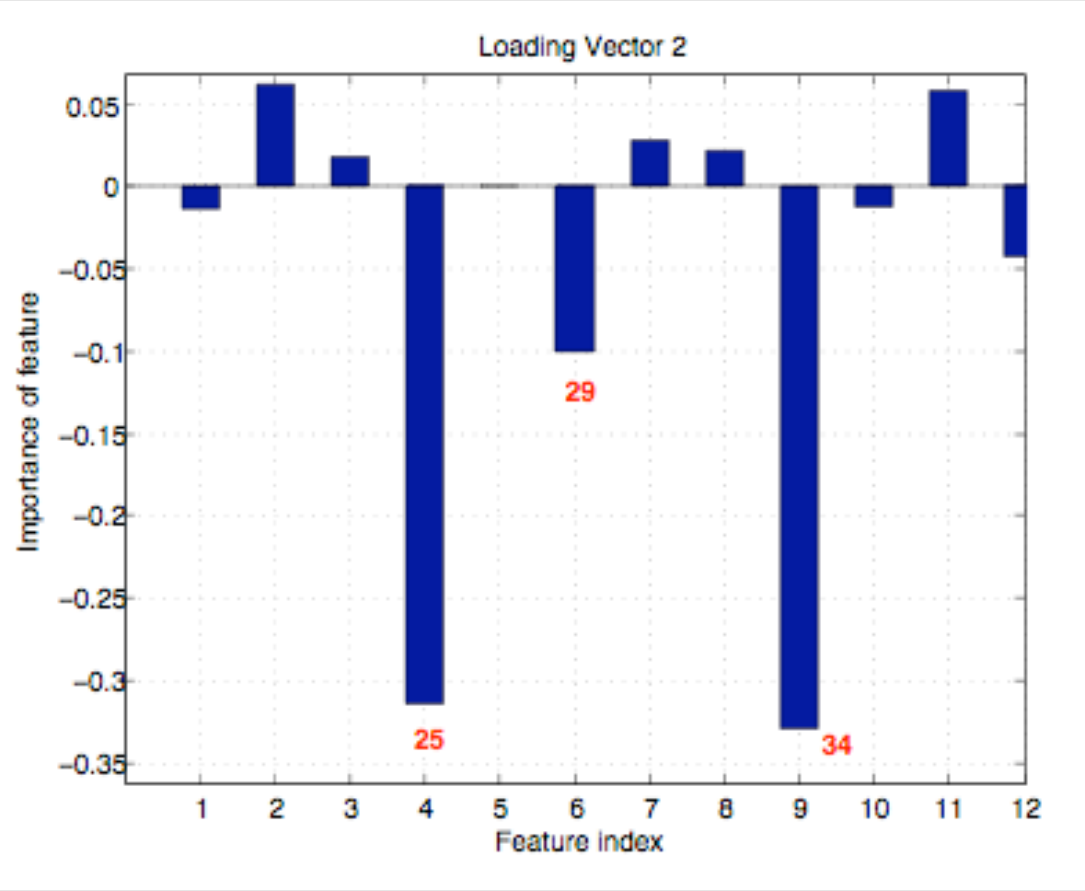
41 lee95_bound




2: trace/norminf,

29: positive fraction of spectrum,

39: commutator norm/ Frobenius norm squared




25: spectrum aspect ratio

29: positive fraction

34: $\mathrm{Re}(\lambda_{\mathsf{min}})/\mathrm{Re}(\lambda_{\mathsf{max}})$

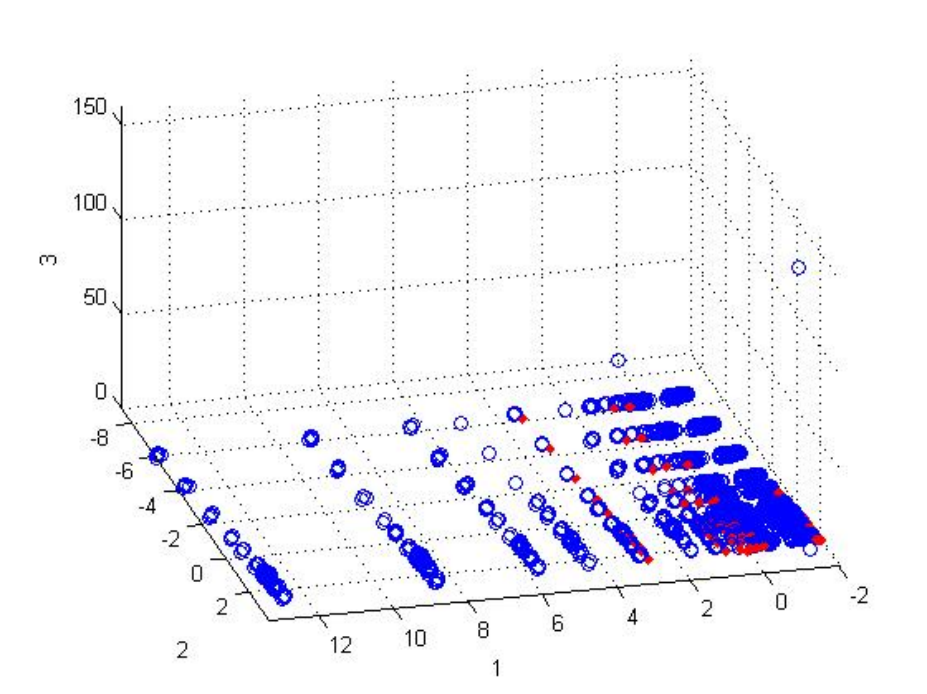
# Overall reliability

single gaussian rate: [0.456790 0.081571 0.830189 1.000000],
sum: 2.368550

kernel mixture rate: [0.901235 0.734139 0.443396 1.000000],
sum= 3.078770

# Speed vs reliability

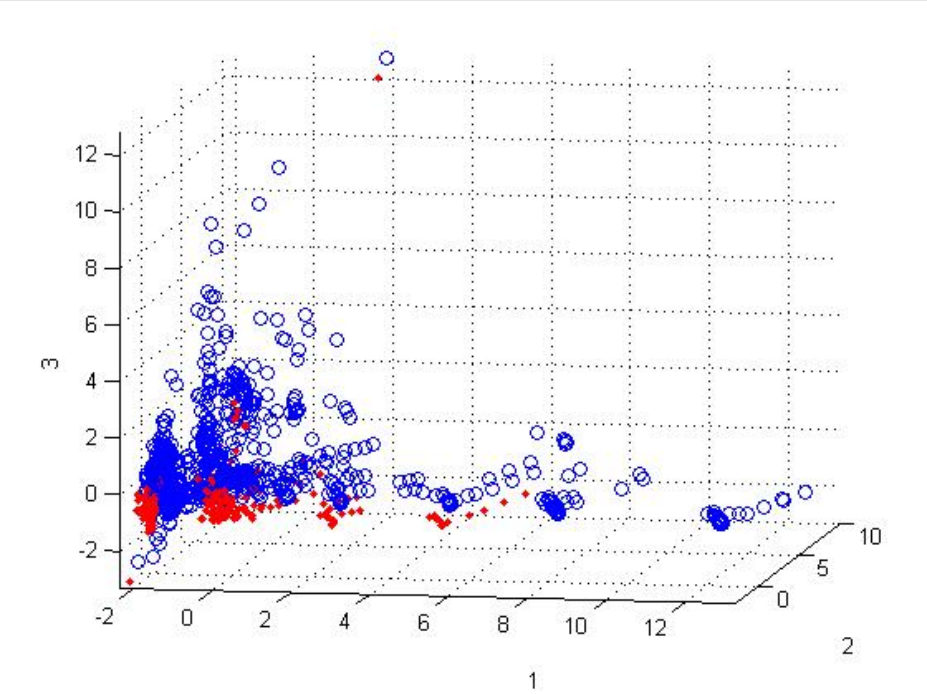
Accuracy figures measure true positives: not always the best measure.
Converge: 93.92%; No-Converge: 56.17%



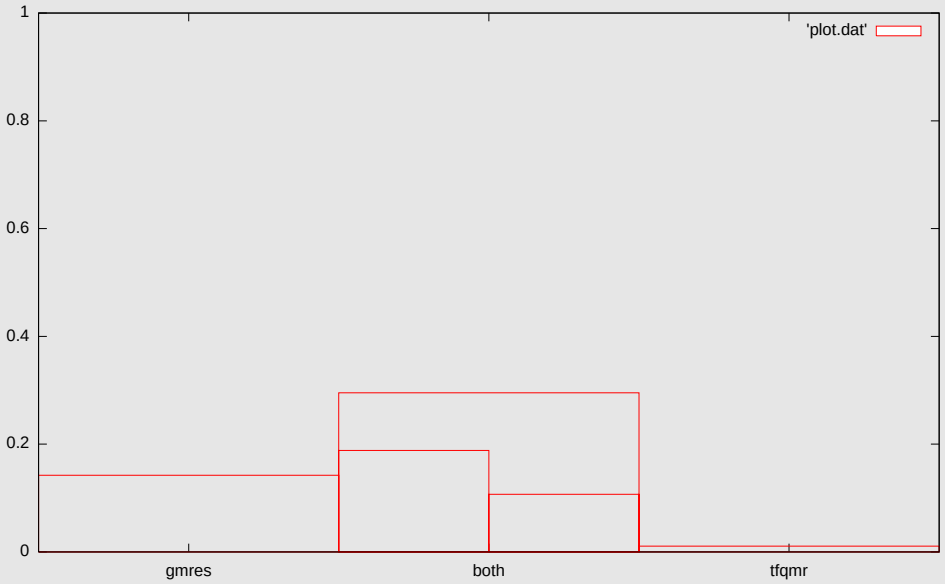

Serious danger of picking non-converging method.
Solution: classify on complement of convergence region, instead of non-convergence

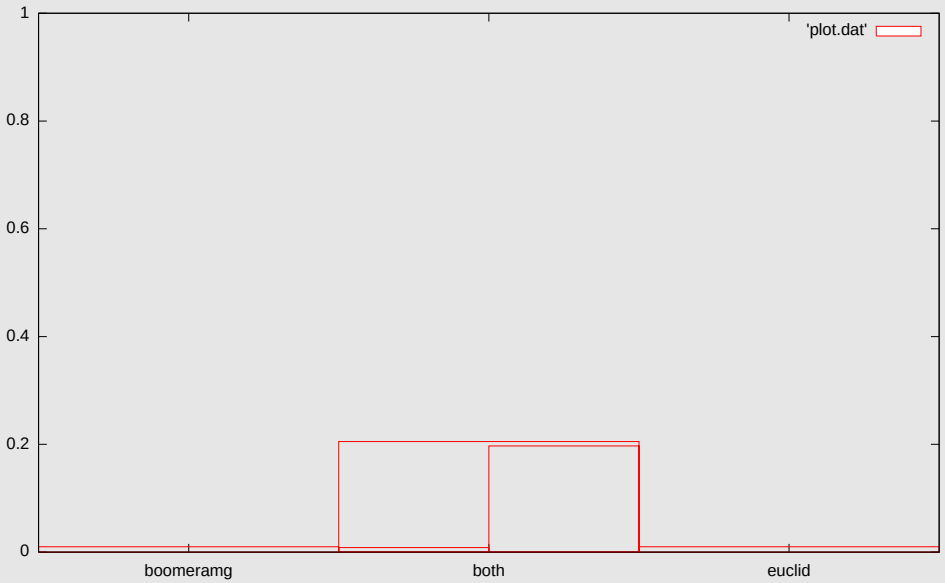
# Order of decisions

Classification of preconditioners easier than of iterators:



# Relative speed and reliability



# Reinforcement learning

# Supervised vs Trial/Error learning

- Bayesian learning is supervised: someone knows the right answer
- Reinforcement learning: by trial and error 'method A is better than B under conditions C'
- Advantages:
  - potentially accurate results with far less work, also easier to update dynamically
  - no database needed: learn through trial-and-error
  - multi-step analysis: possible to pin-point source of error (iterator, preconditioner, etc)

# Reinforcement learning

- Related to Dynamic Programming
- Problem formulated as stochastic shortest path problem (states, actions, instantaneous and final reward)
- Policy is determined through experience: running simulator

# RL for linear solvers

- Stages: pick load distribution, scaling, preconditioner, iterative solver
- Reward: negative of setup and solve time
- State space is divided in overlapping 'tiles'

# RL math

.

- Bellman optimality

$$R(i) = \max_{a \in A(i)} \left[ r(i,a) + \sum_{j \in S} p(i,a,j) R(j) \right]$$

- Q-factor for state-action pair $(i, a)$:

$$Q(i,a) = \sum_{j \in S} p(i,a,j)[r(i,a,j) + R(j)]$$

  then $R(i) = \max_{a \in A(i)} Q(i,a)$

- Observation: $Q(i,a)$ is the expectation of a random variable

# Q-learning

- Now use Robbins-Monro algorithm:

$$E[X] = \lim_{n\to\infty} (1/n) \sum_{i}^{n} s_i = \lim_{n\to\infty} X^n$$

then

$$X^{n+1} = (1 - \alpha^{n+1})X^n + \alpha^{n+1} s_{n+1}, \qquad \alpha^n = 1/n$$

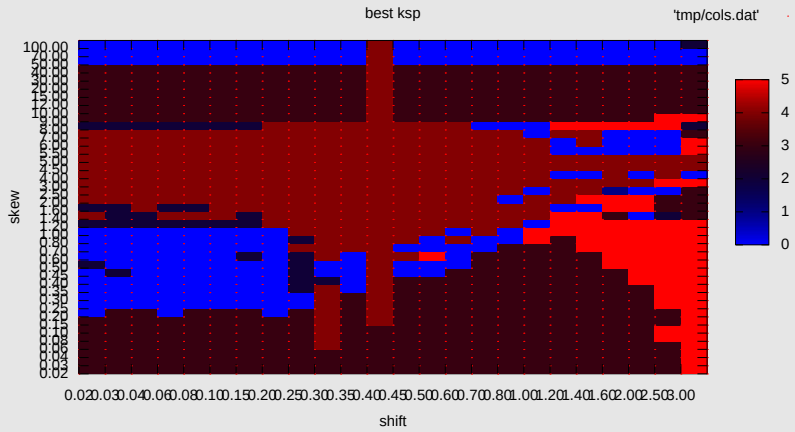
- Q-learning:

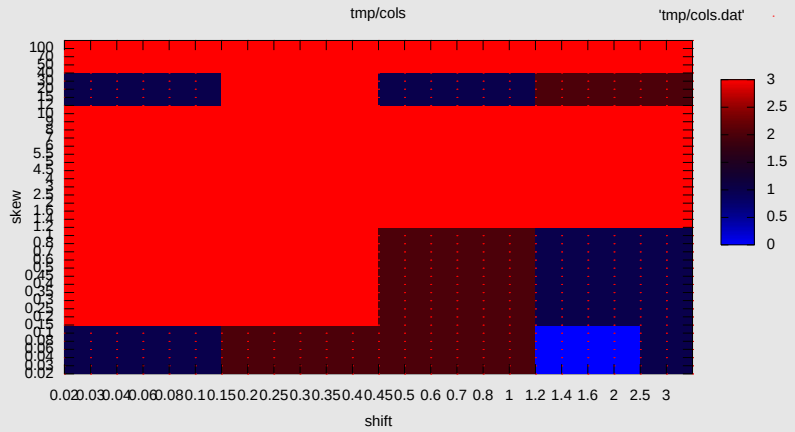
$$Q^{n+1}(i,a) \leftarrow (1-\alpha^{n+1})Q^n(i,a) + \alpha^{n+1} \left[ r(i,a,j) + \max_{b \in A(j)} Q^n(j,b) \right]$$

- Note: no probabilities! This can be run through a simulator.

# Test of Reinforcement Learning

## Best vs Recommended:




- Picks the right method in less than 60% of the cases
- however, in 95% is within 5% of optimal time.
- Possible spread can over 50×

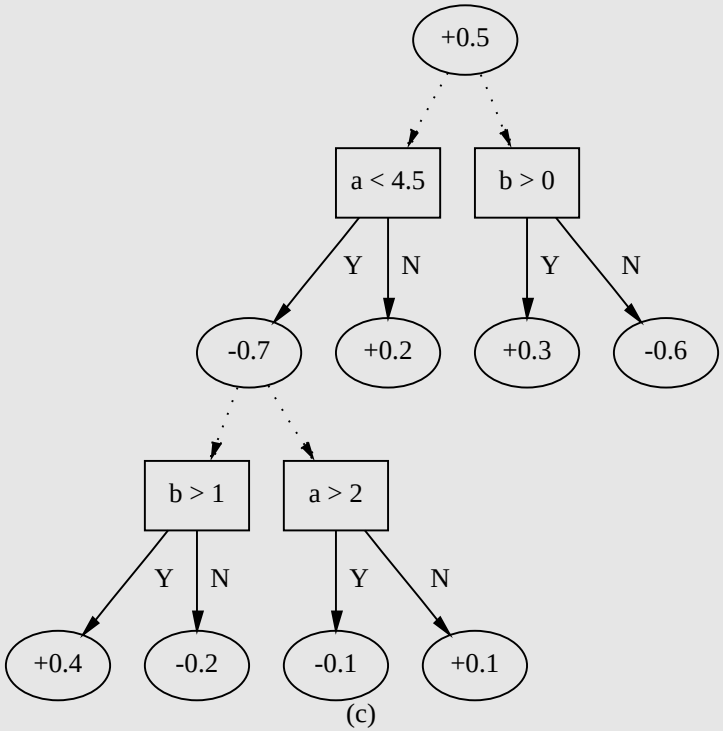
# Boosting

# Abstract formulation of machine learning

Binary classification rule maps instance space $\mathbb{A} \times \mathbb{M} \mapsto \{0, 1\}$
(equivalent to earlier $\mathbb{A} \mapsto \mathbb{M}$)
Without definition: weak PAC learning, strong PAC learning,
Boosting turns weak learning algorithm into strong.

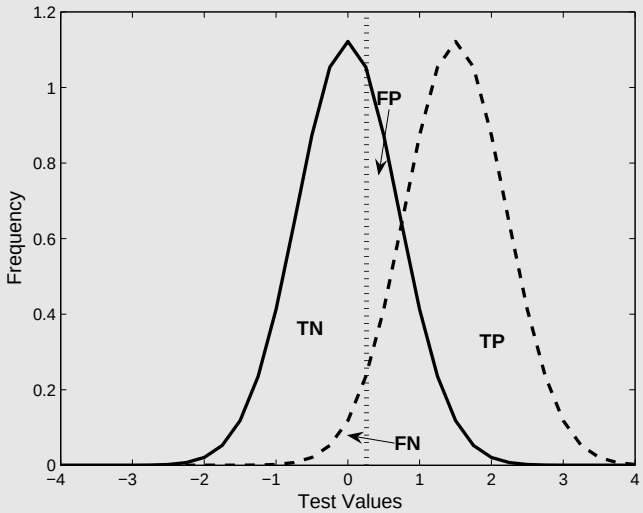
# Alternating decision trees

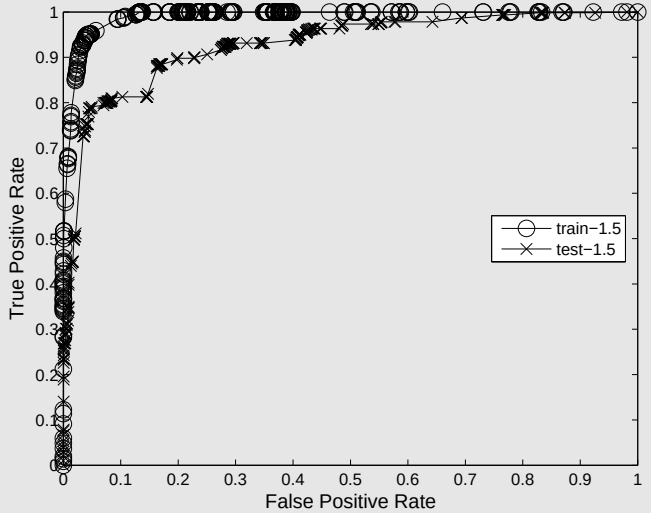
## Use as weak learner (MLJava package)



# Binary classification

Decision: does the method work faster than some reference method
Measurement by ROC curves:



# Conclusions and future work

- Software system: underway to a modular setup
- Bayesian: high reliability;
  to explore: combinations of steps
- RL: promising;
  to explore: more irregular test data, more adaptive algorithm
- Boosting: also promising;
  to explore: classification of reliability; prediction of components seperately.
- In general: non-model test data, more method choices, put all the pieces together.
- Integration in Petsc...
- Release of all software (`http://icl.cs.utk.edu/salsa`)