Numerical tensor methods and their applications

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14 May 2013

All lectures

4 lectures,

- 2 May, 08:00 - 10:00: Introduction: ideas, matrix results, history.
- 7 May, 08:00 - 10:00: Novel tensor formats (TT, HT, QTT).
- 8 May, 08:00 - 10:00: Advanced tensor methods (eigenproblems, linear systems).
- 14 May, 08:00 - 10:00: Advanced topics, recent results and open problems.

Brief recap of Lecture 3

- QTT-format: explicit representations of functions
- QTT-format: explicit representation of operators
- QTT theorem
- QTT-Fourier transform as a tensor network
- QTT-convolution
- Linear systems
- Eigenvalue problems

Plan of lecture 4

- Dynamical low-rank approximation
- Solving non-stationary problems
- Solving multiparametric problems
- Applications to multiparametric problems

Non-stationary problems

Basic setting:

$$\frac{dy}{dt} = F(y,t), \quad y(0) = y_0$$

$$y \to Y(i_1, \ldots, i_d)$$

Application: spectra

Of the main application is the computation of
vibrational spectra

Application: spectra

Problem setting:

$$\frac{d\psi}{dt} = iH\psi, \quad \psi(0) = \psi_0.$$

- $\psi = \psi(q_1, \ldots, q_f)$ — wavefunction
- $H = -\frac{1}{2}\Delta + V(q_1, \ldots, q_f)$.
- $\Delta = \sum_{i=1}^{f} \frac{\partial^2}{\partial q_i^2}$.
- V — potential energy surface
- $q_1, \ldots, q_f$ — degrees of freedom

Application: spectra

Initial setting is the Scrödinger equation

1. Fix the positions of the nuclei — get the energy $V(R_1, \ldots, R_N)$
2. Find the minima, expand V again the minima into Taylor series.
3. (optional): Find normal coordinates, $f = 3N - 6$ (N is the number of atoms)

Main equation

$$\frac{d\psi}{dt} = i(-\frac{1}{2}\Delta + V)\psi, \quad \psi(0) = \psi_0.$$

Discretize on a grid. Laplace has TT-ranks equal to 2 and QTT-ranks bounded by 4.

Main equation

What about V?

Theorem (Rank estimate)

For the polynomial of form

$$V(q_1, \ldots, q_f) = \sum_{i_1, \ldots, i_s = 1}^{f} a(i_1, \ldots, i_s) \prod_{k=1}^{s} q_{i_k},$$

$$\mathbf{rank}_{TT}(V) = C_0 f^{[\frac{s}{2}]} + o(f^{[\frac{s}{2}]}).$$

Main equation

$$\frac{d\psi}{dt} = i(-\frac{1}{2}\Delta + V)\psi, \quad \psi(0) = \psi_0.$$

Discretize on a grid. Laplace has TT-ranks equal to 2 and QTT-ranks bounded by 4.
It is easy to put $H = -\frac{1}{2}\Delta + V$ into the TT-format.

But how it is connected to the computation of spectra?

Eigenvalues via spectra

We want to compute:

$$H\psi = \lambda\psi,$$

But what we do:

1. Take some ψ_0
2. Solve $\frac{dpsi}{dt} = H\psi, \quad \psi(0) = \psi_0.$
3. Compute \$a(t) = (\psi(t), \psi(0))
4. Find FFT of $a(t)$.

Eigenvalues via spectra

$$\psi(t) = \exp(iHt)\psi_0$$

$$\psi_0 = \sum_{k=0}^{\infty} c_k \phi_k,$$

$$H\phi_k = \lambda_k \phi_k,$$

$$a(t) = \sum_{k=0}^{\infty} |c_k|^2 \exp(i\lambda_k t)$$

Thus, the FFT of $a(t)$ gives pikes at λ_k (try that!)

Why should you do that?

Eigenvalues via spectra

How to select initial condition?

$$\psi_0 = \sum_{k=0}^{\infty} c_k \phi_k,$$

c_k should not decay fast!

Example: harmonic oscillator,

Typically $\psi_0 = \prod_{k=1}^{f} \exp(-\alpha_k (q_k^{(0y)} - q_k)^2)$.

Problems and solutions

$$\frac{d\psi}{dt} = i(-\frac{1}{2}\Delta + V)\psi, \quad \psi(0) = \psi_0.$$

It is a hyperbolic problem ($\approx$ square root of the wave equation)

The ranks grow with $t \longrightarrow \infty$ (can become chaotic, boundary reflections, etc.)

No chance?

Dynamical approximation

The idea of the dynamical approximation: replace $\psi(t)$ by its low-parametric representation $\widehat{\psi}(t)$ and hope that $a(t)$ has the same statistics

How to find $\psi(t)$?

Dynamical approximation

The idea of the dynamical approximation: replace $\psi(t)$ by its low-parametric representation $\widehat{\psi}(t)$ and hope that $a(t)$ has the same statistics

How to find $\psi(t)$?

We need an optimization principle

The answer: Dirac-Frenkel variational principle!

Manifold

S Holtz, T Rohwedder, R Schneider - Numerische Mathematik, On manifolds of tensors of fixed TT-rank

The set of tensors with bounded TT-ranks forms a manifold

$$\mathrm{TT}_{\mathbf{r}}, \quad \mathbf{r} = (r_1, \ldots, r_{d-1})$$

Tangent space

We can define a tangent space $\mathcal{M}(\mathbf{TT_r})$ at a point X

Do it only in 2D (C. Lubich)

$$A = USV^\top$$

$$\delta A = \delta U S V^\top + U \delta S V^\top + U S \delta V^\top$$

Projector onto the tangent space:

$$P_X(\delta A) = \delta A - (I - UU^\top)\delta A (I - VV^\top)$$

Tangent space(2)

Why should we care about the tangent space?

Because of the variational principle

Dirac-Frenkel

Given $A(t)$, the dynamical (low-rank) approximation is defined as $X(t)$

$$(\frac{dA}{dt} - \frac{dX}{dt}, \delta X) = 0, \quad \delta X \in \mathcal{T}_X(\mathcal{M})$$

The velocity is in the tangent space!

Dynamical low-rank appr. of matrices

The equations for U, S, V:

$$\frac{dU}{dt}(t) = (I - U(t)U(t)^\top)\frac{dA}{dt}(t)V(t)S(t)^{-1}$$
$$\frac{dV}{dt}(t) = (I - V(t)V(t)^\top)\frac{dA}{dt}(t)^\top U(t)S(t)^{-\top}$$
$$\frac{dS}{dt}(t) = U(t)^\top \frac{dA}{dt}(t)V(t).$$

Dynamical low-rank appr. of matrices

$$\frac{dX}{dt} = P_X\left(\frac{dA}{dt}\right)$$

MCTDH

MCTDH (H.-D. Meyer)

MultiConfigurational Time-dependent Hartree Method

Uses dynamical low-rank approximation in the Tucker format!

Equations for the factors, equations for the core

How to integrate them well?

Problems with dynamical low-rank integration

The main problem of the dynamical equations is the inversion of S

But the equation for X does not have this problem!

$$P_X(Z) = Z - (I - UU^\top)Z(I - VV^\top)$$

KSL integrator

C. Lubich, O., Projector-splitting integrator for the dynamical low-rank approximation of matrices

Splitting

$$P(Y)Z = ZP_{\mathcal{R}(Y^\top)} + P_{\mathcal{R}(Y)}Z - P_{\mathcal{R}(Y)}Z$$

Algorithm:

- K-step: $\frac{d(US)}{dt} = \frac{dA}{dt}V$
- QR: $K_1 = U_1\widehat{S}_1$
- L-step: $\frac{d(VS^\top)}{dt} = \frac{dA}{dt}^\top U$
- QR: $L_1 = U_1\widetilde{S}_1$
- S-step: $\frac{dS}{dt} = -U^\top\frac{dA}{dt}V$ (backward in time!)

Splitting

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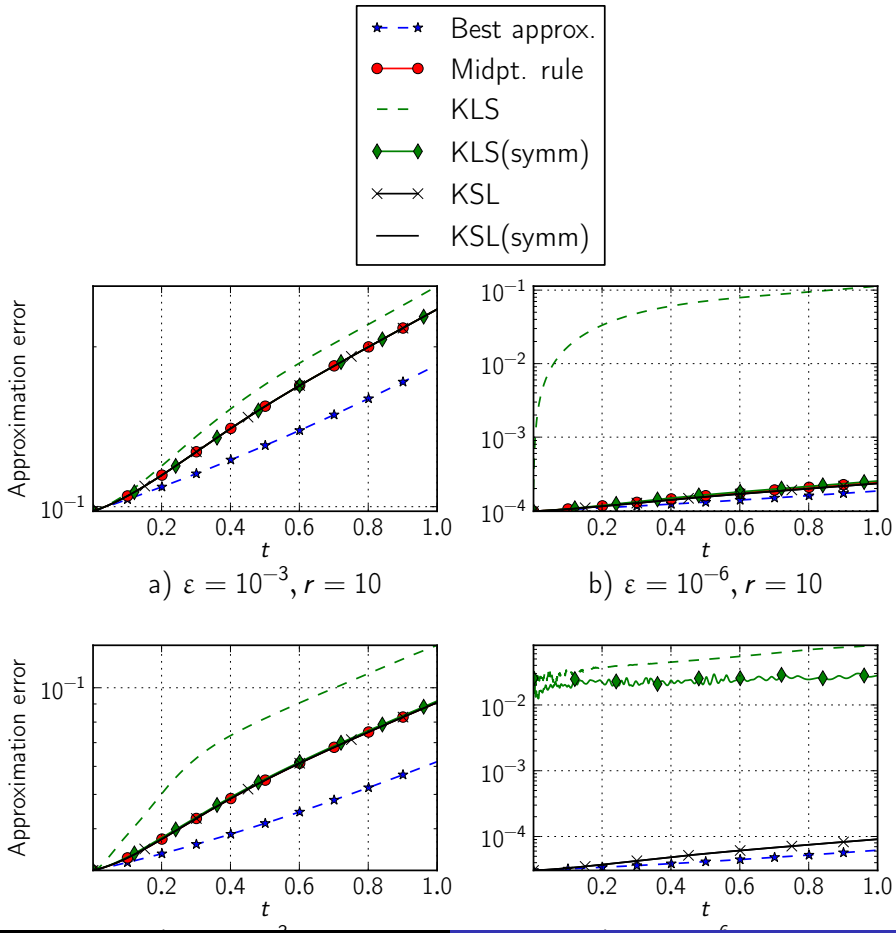
First order explicit scheme, KLS

Splitting

The K-S-L ordering is much better

Experiments on rank-10 matrix A with noise ε.



Theory

Theorem (Exactness)

Suppose that $A(t)$ has rank at most r for all t. With the initial value $Y_0 = A(t_0)$, the splitting algorithm is then exact: $Y_1 = A(t_1)$.
From this fact we can prove overapproximation result

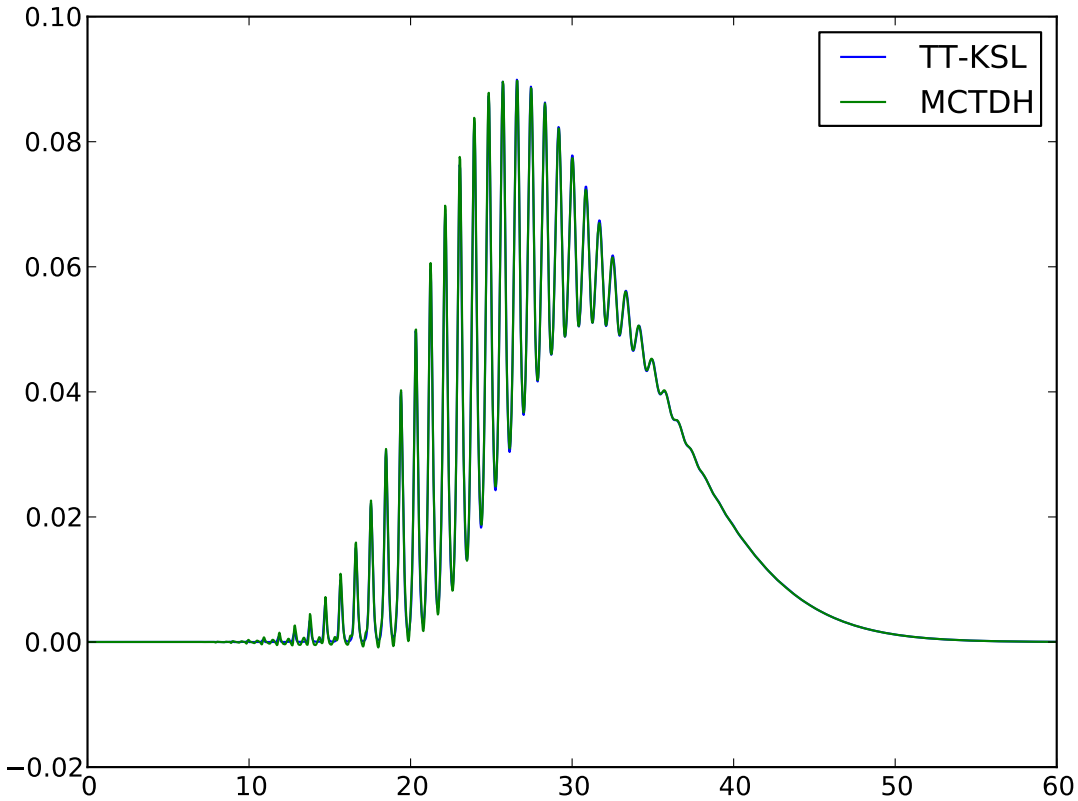
Multidimensional case

- The extension to HT/TT format is (almost done)
- The extension to $\frac{dy}{dt} = Ay$ is done
- The integrator can be readily applied to optimization problems (project the gradient/Newton step)
- Implemented in **ttpy** package (http://github.com/oseledets/ttpy)
- The CECAM workshop: C. Lubich, B. Vandereycken, R. Schneider, I. Oseledets talks

Comparison with MCTDH

$$V(q_1, \ldots, q_f) = \frac{1}{2}\sum_{k=1}^{f} q_k^2 + \lambda \sum_{k=1}^{f-1} \left(q_k^2 q_{k+1} - \frac{1}{3} q_k^3\right).$$

http://www.pci.uni-heidelberg.de/cms/mctdh.html



Other techniques

There are other important techniques for non-stationary problems

DG

V. Kazeev, O. Reichmann, Ch. Schwab

Discontinious Galerkin in time:

Leads to shifted linear systems

$$(A - \lambda_i I) u_i = f$$

- DMRG/AMEN solvers, estimates
- Non-symmetric problems (can be harsh)

Block time scheme

Time as a dimension:

O., S. Dolgov, B. Khoromskij

Block time scheme

Time as a dimension:

O., S. Dolgov, B. Khoromskij

Consider an Euler scheme:

$$y_{k+1} = (I - \tau A) y_k = S y_k$$

Write as big linear system with $N \times T$ unknowns:

$$(I \otimes Z - S \otimes I) Y = f$$

Take $T = 2^d$.

Apply DMRG/AMEN!

Open questions

Several open questions

- How to adapt the rank
- "Stable" low-rank parametrization (U, S, V is bad)!
- Estimates for the projected methods

Multiparametric problems

One of the most interesting applications — solution of multiparametric problems

$$A(p)u(p) = f(p)$$
$$A(p) : \mathbb{R}^N \to \mathbb{R}^N$$
$$p = (p_1, \ldots, p_M)$$

Multiparametric problems

After discretization, we are left with a huge linear system

$$\mathbb{A}u = f,$$

where u is $N \times P \times \ldots \times P$ — a tensor!

Tensor-structured linear system

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$$A = A_0 + A_1 p_1 + A_2 p_2 + \ldots A_M p_M$$

$$\mathbb{A} = I + I \otimes D \otimes I + \ldots$$ — rank M.

Tensor-structured linear system

Matrix format, no CP requirements

$$\mathbb{A} \approx A_1(i_1, j_1) A_2(i_2, j_2) \dots A_d(i_d, j_d).$$

How to solve multiparametric problems

What about multiparametric problems?
Can not apply DMRG/AMEN directly
One mode (first one) is large

How to solve multiparametric problems

Idea is to combine with model reduction techniques (POD, Global POD)

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$$u = Uz$$

Then:

$$A(p)u(p) = f(p) \text{ -> } U^{\top}A(p)Uz(p) = f(p)$$

(Galerkin projection).

This system is much smaller, and can be solved by dmrg_solve

We do not know the basis in advance!

How to solve multiparametric problems

Maxvol-ALS iteration:

- Know the U basis -> solve the reduced problem for $z(p)$.
- Find maximal volume p^*
- Compute new snapshots at these points
- Cycle until convergence

How to solve multiparametric problems

Suppose the separation rank between x and p is r:

$$u(x,p) \approx \sum_{\alpha=1}^{r} U(x,\alpha) Z(\alpha,p)$$

The solution can be recovered from values in r physical points!

Diffusion equation

4-parameter problem

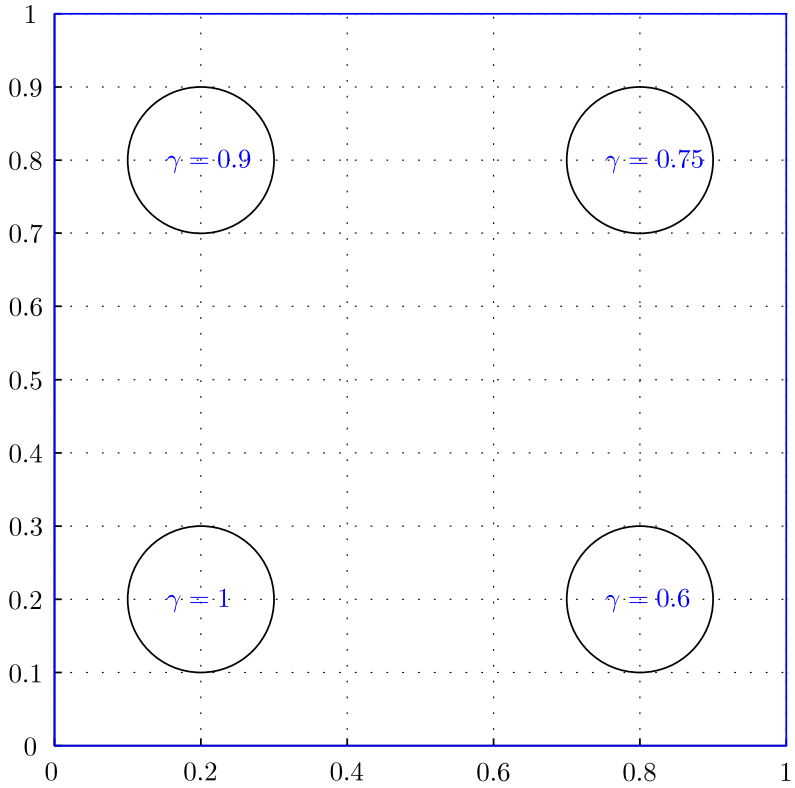
Precision: $\sim 10^{-5}$

Grid: 256×256

S. Galerkin: $\sim \times 100$ larger system

S. Collocation: ~ 1000 more solvers

DMRG + QTT: ~ 100 solves



Instead of $256^2 \times 128^4 = 2^{44}$ we have

around 50000 parameters.

Open questions

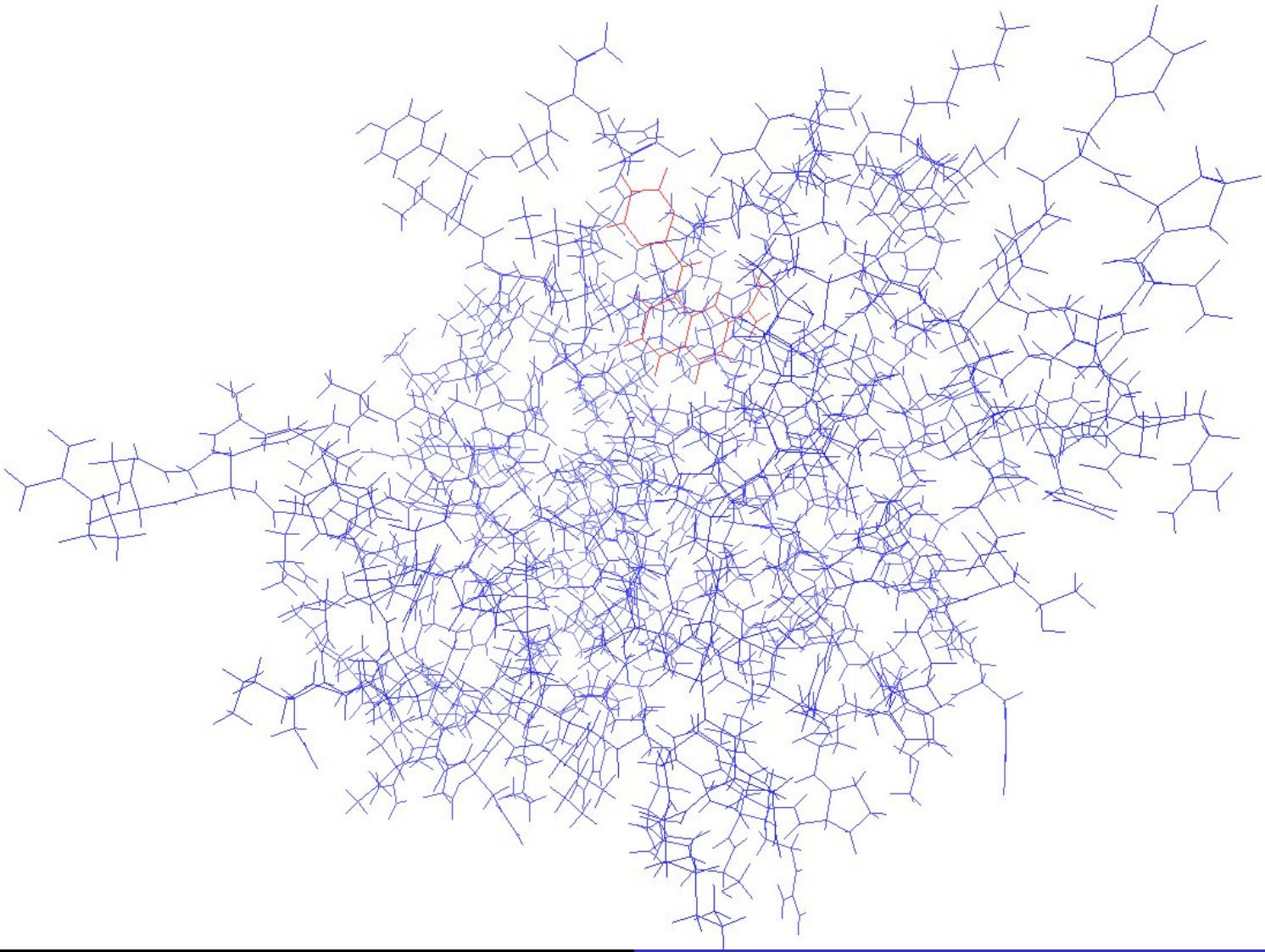
- What class of problems is tractable
- Compare with other techniques (DEIM, sparse grids)
- Efficient numerical implementations are still lacking

Problem of global optimization

It is natural to apply to the problems of global optimization

Protein-ligand

Drug design:



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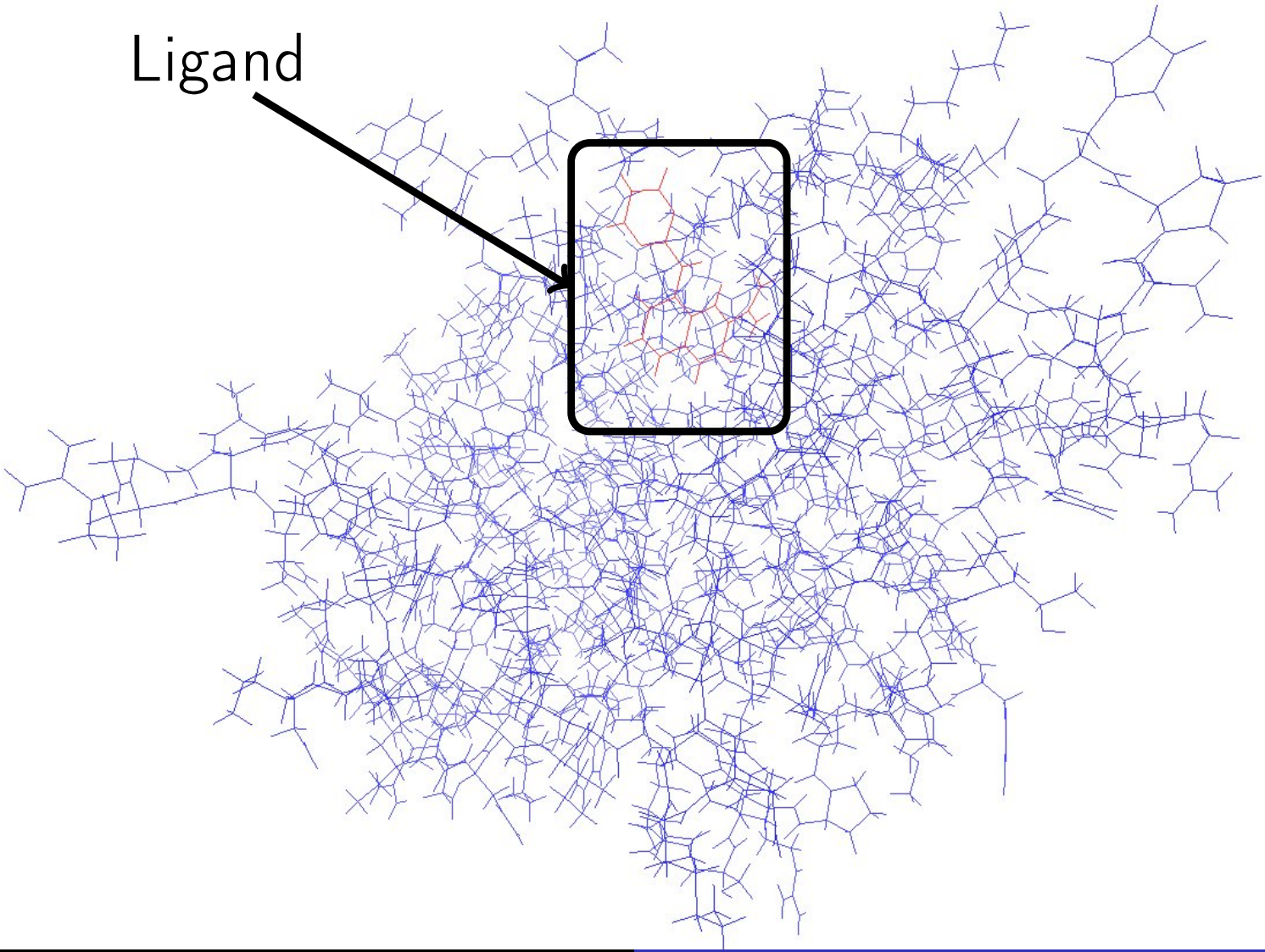

Problem statement

D. Zheltkov

Drug design, 9-variable function

Many local minima, singularities

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Drug design, 9-variable function

Many local minima, singularities

Need global minimum.

Problem statement

$$f(x_1, \ldots, x_d) \longrightarrow \min$$

Use cross approximation:

Problem statement

$$f(x_1, \ldots, x_d) \to \min$$

Use cross approximation:

Use magic transform: $\widehat{f} = \operatorname{arcctg} f$

Results

	Min	Max	Average
Fun calls	18804158	26272810	$2.39 * 10^7$
Min value	-65.1472	-52.7327	-62.9526
Mean val dev., Å	0.666	2.656	0.954
Mean val dev., Å	0.064	2.758	0.474

(All points — 10^9)

Results

np	8	16	32	64	128
Time, c	4834.6	2497.2	1288.1	657.93	336.12
Speedup	7.85	15.2	29.4	57.6	113

Open questions

Open questions:

- Theoretical justification (we have in two dimensions)
- Testing and applications

Latent variable models

A very interesting application:

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Observed variables $S_1, \ldots, S_N$ (stock prices)

There are latent variables.

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latent variable models

Observed variables $S_1, \ldots, S_N$ (stock prices)

There are latent variables.

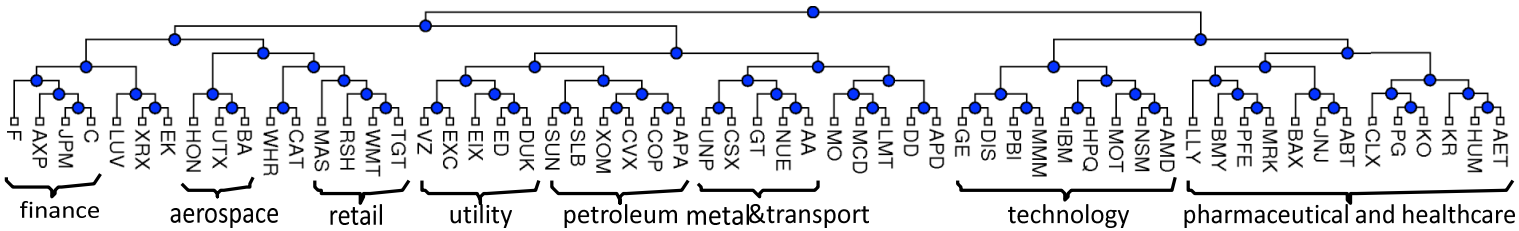
$$p(x_1, x_2) = \sum_{\alpha=1}^{r} p_1(x_1, h) w(h) p_2(x_2, h)$$

You can use tensors! (Ishteva, Le Song, Georgia Tech.)

Latent variable models

Latent tree reconstruction

(M. Ishteva, Le Song)



Open problems

- Test the effectiveness of latent tree detection techniques (Ishteva et. al work is based on a greedy algorithm, MPS people have another approach)
- Approximation of tensors with approximate entries, only through matrix-by-vector products

Hastings area law

- An area law for one dimensional quantum systems, M. B. Hastings
- An improved 1D area law for frustration-free systems, Itai Arad, Zeph Landau, Umesh Vazirani

Area law

If H is $H = \sum_{i=1} H_i$, H_i is 2-local interaction, and H has a spectral gap ε. Then, the ground-state wavefunction can be approximated in the TT (MPS) format. Entropy bound:

$$S_{1D} \leq \mathcal{O}(1) X^3 \log^8 X, \quad X = \frac{J \log d}{\varepsilon}, \quad \|H_i\| \leq J$$

Idea of the proof

The proof is linear algebra!

$H = \sum_i Q_i, \quad P_i = I - Q_i$ — projectors.

Need to estimate the TT-ranks

Idea of the proof

Idea: Find an operator K:

1. $K\psi = \psi$ for a ground-state
2. $\|K\psi_\perp\| \leq \Delta \|\psi_\perp\|$
3. $\mathbf{rank}(K\psi) \leq D\mathbf{rank}(\psi)$
4. $D\Delta \leq \frac{1}{2}$

Then, we can take any rank-1 function apply K and truncate to rank-1.

The overlap will decrease until $\sqrt{\frac{1}{2D}}$.

Idea of the proof

Constucting the operators:

$$\Pi_{even} = P_2 P_4 \ldots, \quad \Pi_{odd} = P_1 P_3 \ldots$$

$A = \Pi_{even}\Pi_{odd}$ is an approximation to the ground-state projection.

- $D_0 = d^2$
- $\Delta_0 \approx 1 - c\varepsilon$.
- $\widehat{A} = \widehat{\Pi}_m \Pi_{even}\Pi_{odd}$
- $\widehat{\Pi}_m = C_m(N)^q, \quad N = \sum_{i=1}^{m}(I - P_i)$, C_m are Chebyshev polynomials

Summary of the course

- Novel tensor formats
- High-dimensional applications (nonstandard ones!)
- Relation to Quantum Information
- A lot of open problems
- Software

Open question

- How to select variables such as they separate?