An experience based guide to Tensorlab

Nico Vervliet

March 3, 2015

Disclaimer

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Optimization

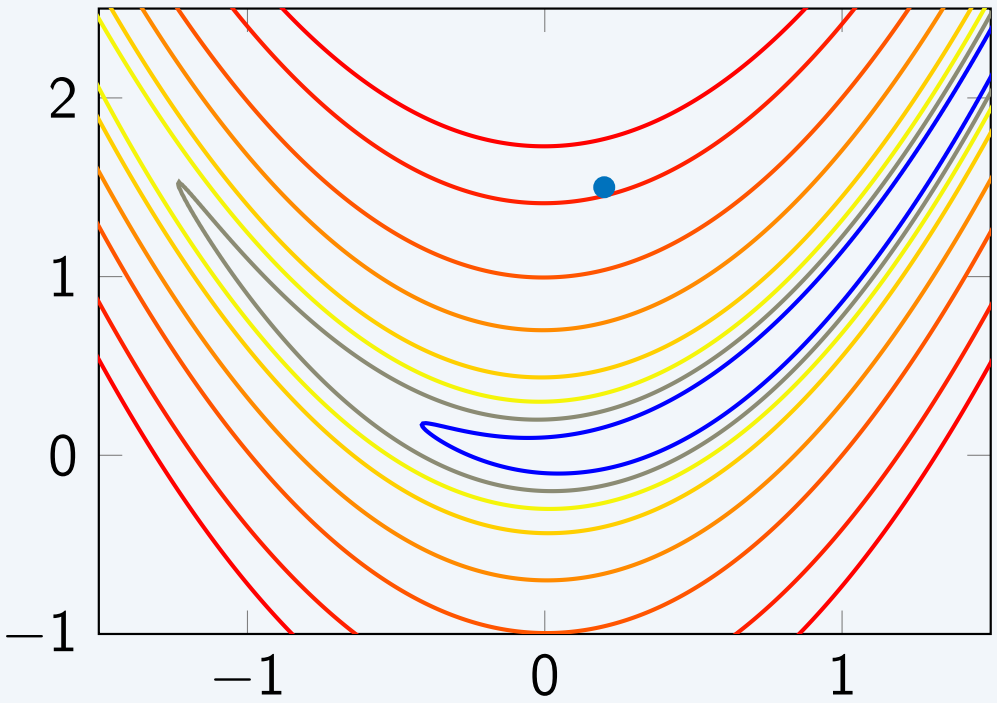
Basics unconstrained optimization

- Find $\mathbf{x}$ that minimizes objective function f:

$$\min_{\mathbf{x}} f(\mathbf{x})$$

- Iteratively update guess $\mathbf{x}_k$:

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k$$



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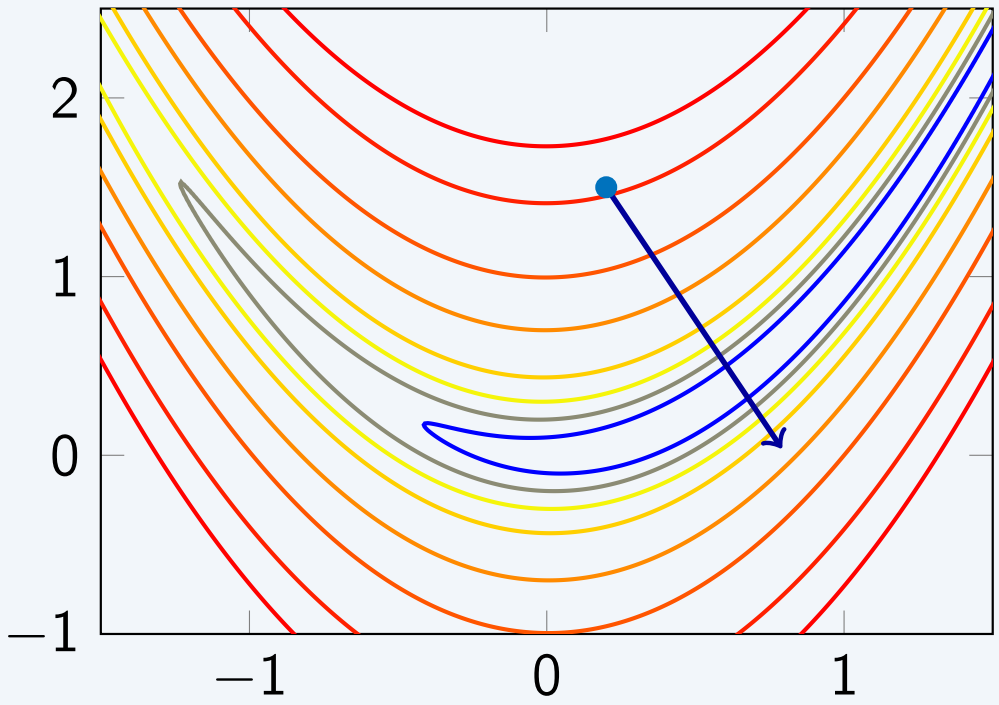

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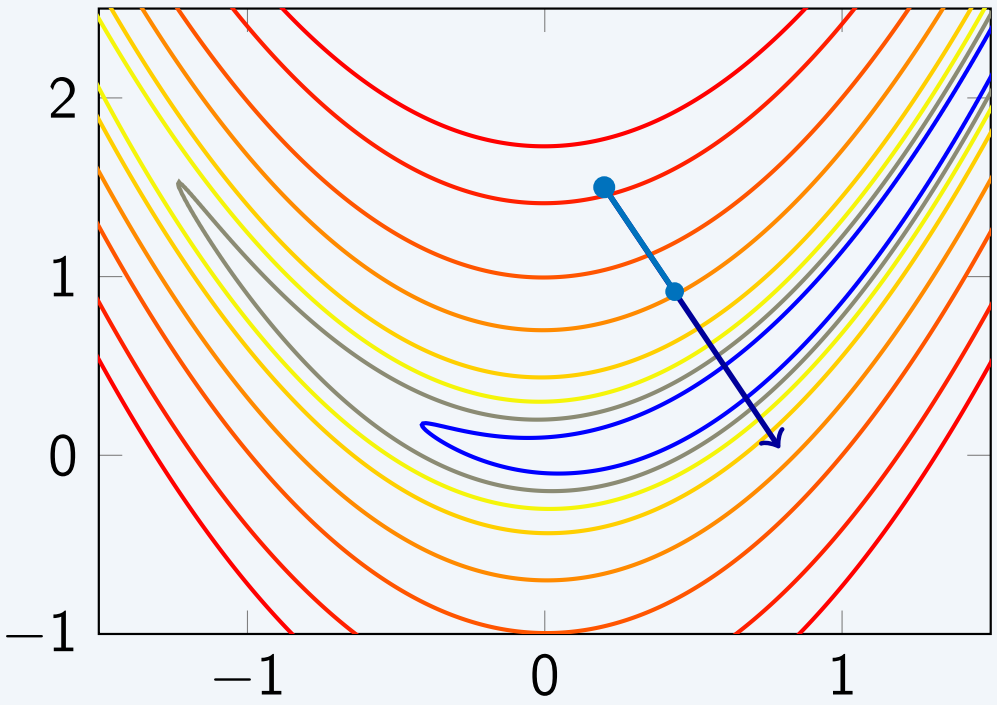

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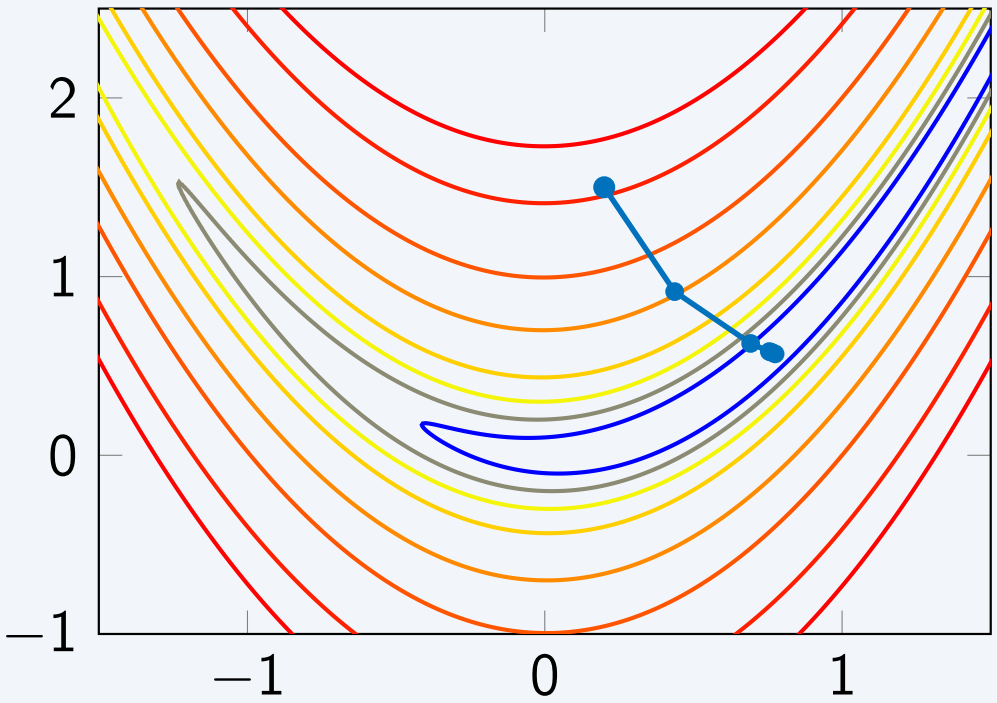
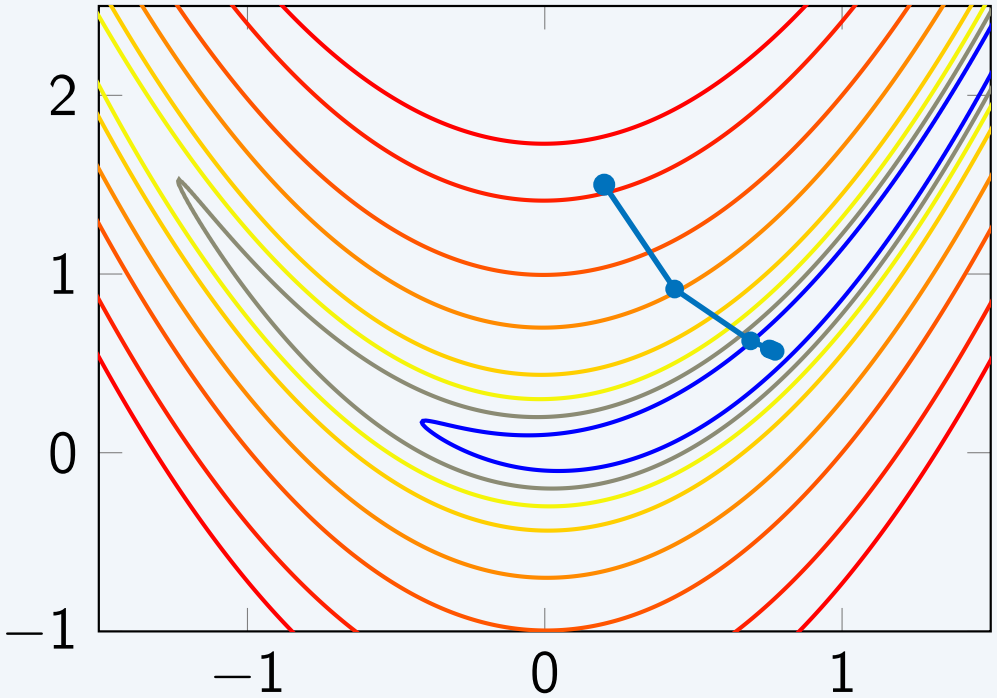


Choosing step direction



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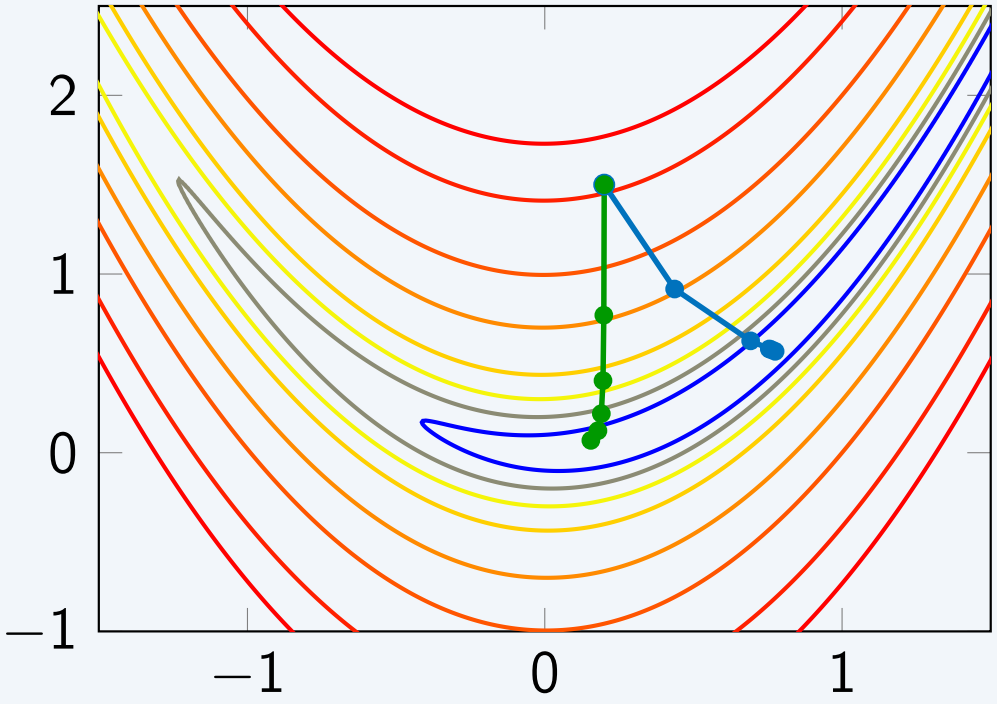

Choosing step direction

- Gradient descent

$$\mathbf{p}_k = -\mathbf{g}_k$$

  - Linear convergence

Choosing step direction

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- Newton

$$\mathbf{p}_k = -\mathbf{H}_k^{-1}\mathbf{g}_k$$

  - Quadratic convergence

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- Newton

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  - Quadratic convergence
- Quasi-Newton

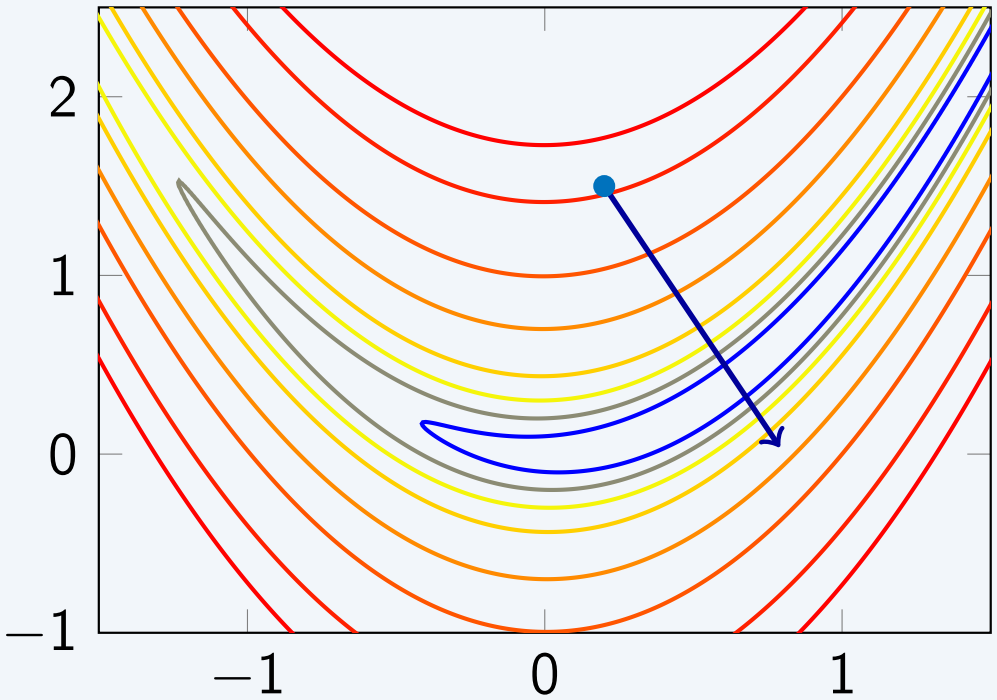
$$\mathbf{p}_k = -\mathbf{B}_k^{-1}\mathbf{g}_k$$

  - Superlinear to quadratic convergence
  - Examples: (L)BFGS, SR1, Gauss–Newton, Levenberg–Marquardt

Choosing step length

- Line search (`cpd_aels`, `cpd_els`, `cpd_lsb`, `ls_mt`)

$$\min_{\alpha_k} f(\mathbf{x}_k + \alpha_k \mathbf{p}_k)$$



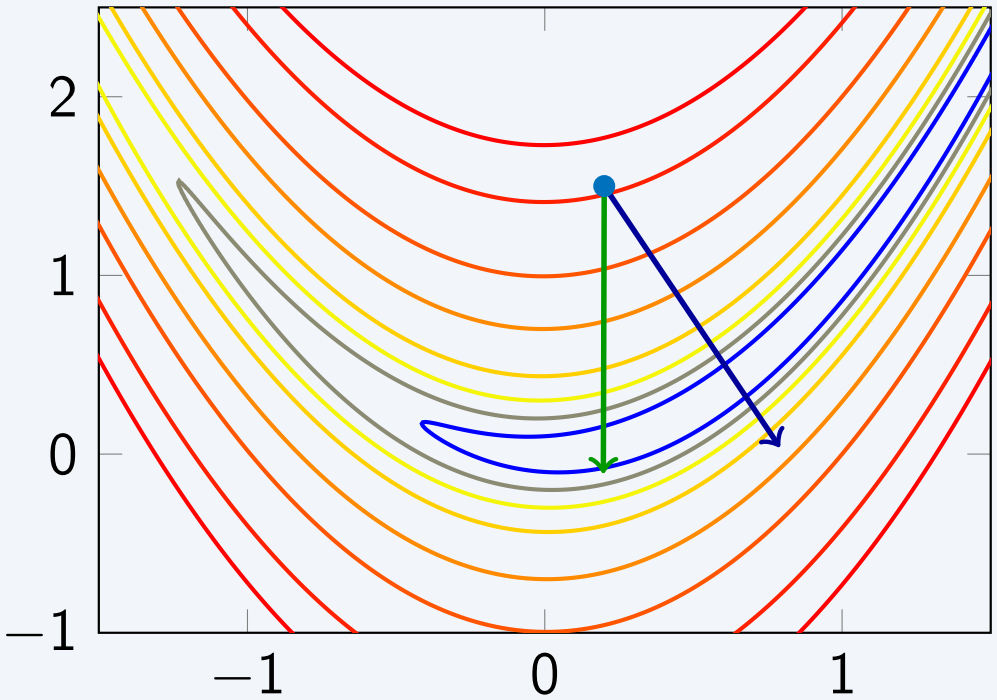
Choosing step length

- Line search (`cpd_aels`, `cpd_els`, `cpd_lsb`, `ls_mt`)

$$\min_{\alpha_k} f(\mathbf{x}_k + \alpha_k \mathbf{p}_k)$$

- Plane search (`cpd_eps`)

$$\min_{\alpha_k, \beta_k} f(\mathbf{x}_k + \alpha_k \mathbf{p}_k + \beta_k \bar{\mathbf{p}}_k)$$

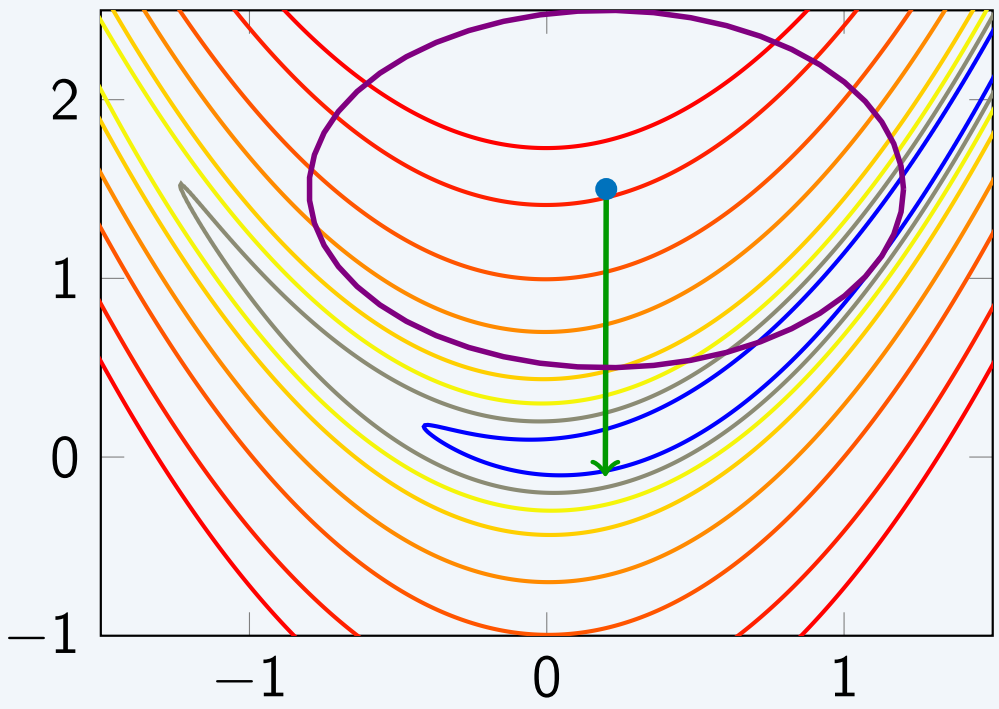


Globalization strategy

- Trust region

$$\min_{\mathbf{p}_k} f_k + \mathbf{g}_k^{\mathsf{H}}\mathbf{p}_k + \frac{1}{2}\mathbf{p}_k^{\mathsf{H}}\mathbf{B}_k\mathbf{p}_k \quad \text{s.t.} \quad ||\mathbf{p}_k|| \leq \Delta_k$$

- Trustworthiness $\rho = (f_k - f_{k+1})/(m_k - m_{k+1})$, m_k is value of quadratic model



Solving systems

Computing $\mathbf{p}_k$ often involves solving

$$\mathbf{B}_k \mathbf{p}_k = -\mathbf{g}_k.$$

The structure of $\mathbf{B}_k$ can often be exploited:

- CG uses only the product $\mathbf{B}_k \mathbf{p}_k$
- Improve convergence using preconditioner (e.g. Block-Jacobi)

$$\mathbf{M}^{-1} \mathbf{B}_k \mathbf{p}_k = -\mathbf{M}^{-1} \mathbf{g}_k.$$

Why?

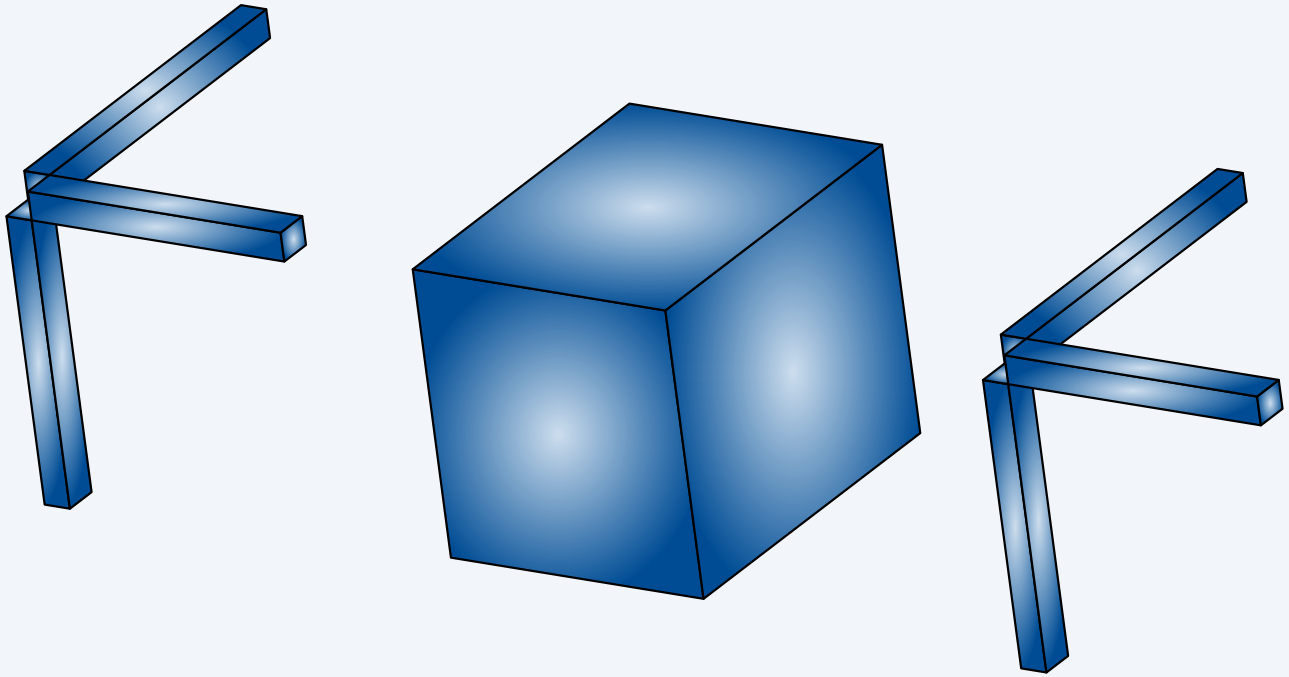
```
    fval                relfval            relstep
    =1/2*norm(F)^2      TolFun = 1e-12     TolX = 1e-06

0:  9.06912804e+05 |
1:  1.60066687e+05 | 8.23503774e-01 | 3.00000000e-01 |

    delta          rho

    1.9076e+01 | 1.0633e+00
```

Options

Control behavior using `options.<...> = ...`:

Parameter	Description
`TolX`	stop if `relstep < TolX`
`TolFun`	stop if `relfval < TolFun`
`MaxIter`	maximum number of iterations
`Display`	display progress every `display` iterations
`PlaneSearch`	plane search algorithm
`Algorithm`	optimization algorithm
`CGMaxIter`	maximum number of CG iterations
`CGTol`	stop if $\|\|\mathbf{B}_k\mathbf{p}_k + \mathbf{g}_k\|\| \,/\, \|\|\mathbf{g}_k\|\| <$ `CGTol`

Canonical Polyadic Decomposition



A nonlinear least squares problem

- A nonlinear, non-convex problem

$$\min_{\mathbf{A},\mathbf{B},\mathbf{C}} \frac{1}{2} ||[\![\mathbf{A},\mathbf{B},\mathbf{C}]\!] - \mathcal{T}||^2$$

A nonlinear least squares problem

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$$\min_{\mathbf{A},\mathbf{B},\mathbf{C}} \frac{1}{2} ||[\![\mathbf{A},\mathbf{B},\mathbf{C}]\!] - \mathcal{T}||^2$$

- How to solve?
  - Alternating least squares: `cpd_als`
  - Quasi-Newton, e.g. (L)BFGS: `cpd_minf`
  - Gauss–Newton or Levenberg–Marquardt: `cpd_nls`

NLS algorithms

The problem

$$\min_{\mathbf{x}} \frac{1}{2} ||\mathcal{F}(\mathbf{x})||^2$$

is linearized around $\mathbf{x}_k$

$$\begin{aligned}\mathcal{F}(\mathbf{x}) &\approx \mathcal{F}(\mathbf{x}_k) + \nabla_{\mathbf{x}}\mathcal{F}(\mathbf{x}_k)(\mathbf{x} - \mathbf{x}_k) \\ &= \mathcal{F}(\mathbf{x}_k) + \mathbf{J}_k\mathbf{p}_k.\end{aligned}$$

Find $\mathbf{p}_k$ that minimizes the quadratic model

$$\mathbf{J}_k^{\mathrm{H}}\mathbf{J}_k\mathbf{p}_k = -\mathbf{J}_k^{\mathrm{H}}\mathbf{g}_k$$

using CG.

Algorithms to choose from

Algorithm	Cost/Iteration	# Iterations	Overal
`cpd_gevd`	n.a.	1	fast
`cpd_als`	cheap	a lot	slow/fast
`cpd_minf`	moderate	not too many	fast
`cpd_nls`	expensive	a few	fastest

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`cpd_nls`	expensive	a few	fastest

- Which algorithm should you use?
  - In general: `cpd_nls`
  - Sometimes `cpd_minf` gives higher accuracy
  - For easy problems: `cpd_als`
  - In noiseless cases and as initialization: `cpd_gevd`

How to get the right solution fast?

How to get the right solution fast?

I don't know...

A strategy

1. Compression
2. Initialization
3. Decomposition
4. Refinement

Compression

- Compute CPD of compressed tensor instead of full tensor to
  - reduce computation time
  - reduce noise

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- Compute CPD of compressed tensor instead of full tensor to
  - reduce computation time
  - reduce noise
- Algorithms:
  - `lmlra_aca`: fast, but not always very accurate (low SNR)
  - `mlsvd`: slow, but very accurate
  - `lmlra_rff`: fast and accurate experimental

Compression: how?

- When using `cpd`:

```
options.Compression = 'auto' % or true or false;
```

Currently only `lmlra_aca`.

Compression: how?

- When using cpd:

```
options.Compression = 'auto' % or true or false;
```

Currently only `lmlra_aca`.

- Manually:

```
[U, S] = lmlra_aca(T, core_size);
[U, S] = mlsvd(T, core_size);
[U, S] = lmlra_rff(T, core_size);
```

Choose `core_size>=[R R R]`.

```
Ures = cpd_nls(S, Uinit, options);
Ures = cellfun(@(u, v) v*u, Ures, U, 'uni', 0);
```

Initialization

A good initial guess is needed for:

- convergence to a (local) optimum
- convergence to a good optimum
- fast convergence

Algorithms:

- `cpd_rnd`
- `cpd_gevd` (when $R \leq I_n$ for at least two n)
- manual (using knowledge)

Initialization: how?

- When using cpd:

```
options.Initialization = 'auto'; % or @cpd_rnd or
                                 % @cpd_gevd
options.InitializationOptions = struct('Imag', @rand);
```

- Manually:

```
Uinit = cpd_rnd(size_tens, R, struct('Real', @rand));
Uinit = cpd_rnd(T, R, 'optimalScaling', true);
Uinit = cpd_rnd(T, R, 'Angle', pi/3);
Uinit = cpd_gevd(T, R);
```

Decomposition

Actually decompose the (compressed) tensor.
Algorithms:

- `cpd_als`
- `cpd_minf`
- `cpd_nls` (preferred)

Decomposition: how?

- When using cpd:

```
options.Algorithm = @cpd_nls; % default
options.AlgorithmOptions = struct(...);
```

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options.AlgorithmOptions = struct(...);
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- Manually:

```
Ures = cpd_nls(S, Uinit, options);
```

- Remark: `options` in `cpd_nls` is `options.AlgorithmOptions` in `cpd`.

Decomposition: options

- Change solver

```
opt.Algorithm = @nls_gndl; % or @nls_lm or @nls_gncgs
opt.Algorithm = @(F, dF, z0, opt) ...
                nlsb_gndl(F, dF, LB, UB, z0, opt);
```

Decomposition: options

- Change solver

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opt.Algorithm = @nls_gndl; % or @nls_lm or @nls_gncgs
opt.Algorithm = @(F, dF, z0, opt) ...
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```

- Change termination criteria

```
opt.TolFun = eps^2; % Rule of thumb: TolX^2
opt.TolX = eps;
opt.MaxIter = 100;
```

Decomposition: options

- Change solver

```
opt.Algorithm = @nls_gndl; % or @nls_lm or @nls_gncgs
opt.Algorithm = @(F, dF, z0, opt) ...
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- Change termination criteria

```
opt.TolFun = eps^2; % Rule of thumb: TolX^2
opt.TolX = eps;
opt.MaxIter = 100;
```

- Change advanced settings (only large scale)

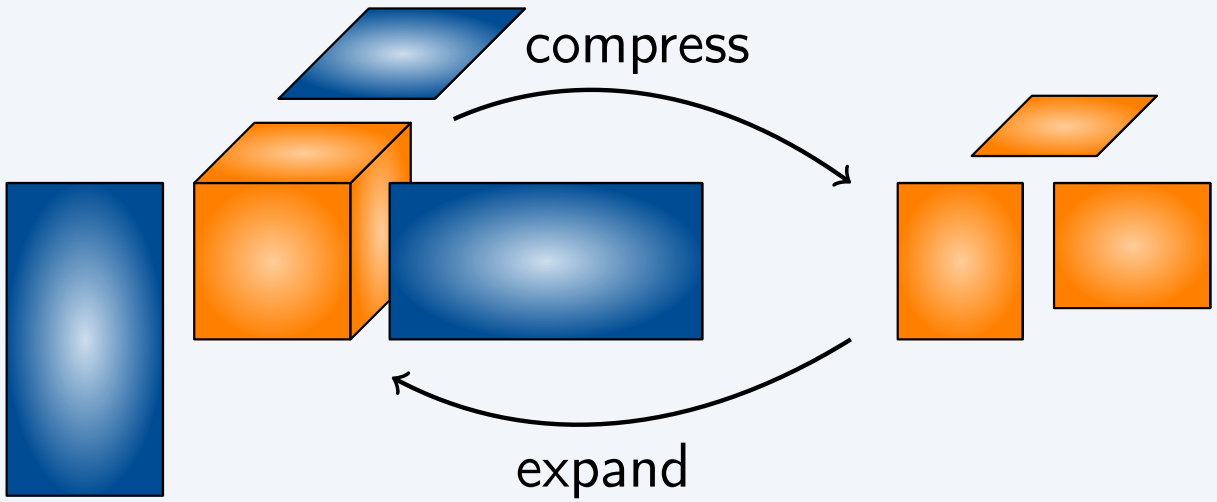
```
opt.CGMaxIter = 10;
opt.CGTol = 1e-6;
```

Higher number of iterations or lower tolerance, decreases # iterations, but increases time per iteration.

Refinement

Use the decompressed solution as initialization for the original tensor (only if compression is used.)

```
% U = factor matrices from compression
% Ures = factor matrices from CPD of core tensor S
Uinit = cellfun(@(u, v) v*u, Ures, U, 'uni', 0);
```



Refinement: how?

- When using cpd

```
options.Refinement = @cpd_nls;
options.RefinementOptions = struct(...);
```

- Manually:

```
Ures = cpd_nls(T, Uinit, struct(...));
```

Estimating the rank

- Use `rankest`
  - Fails on very noisy tensors
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  - Check fit:

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```

  - Check factor matrices (if original are known):

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cpderr(Ures, U0)
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  - Look for degenerate terms (sums of terms that cancel each other out)
  - Use measures from your field

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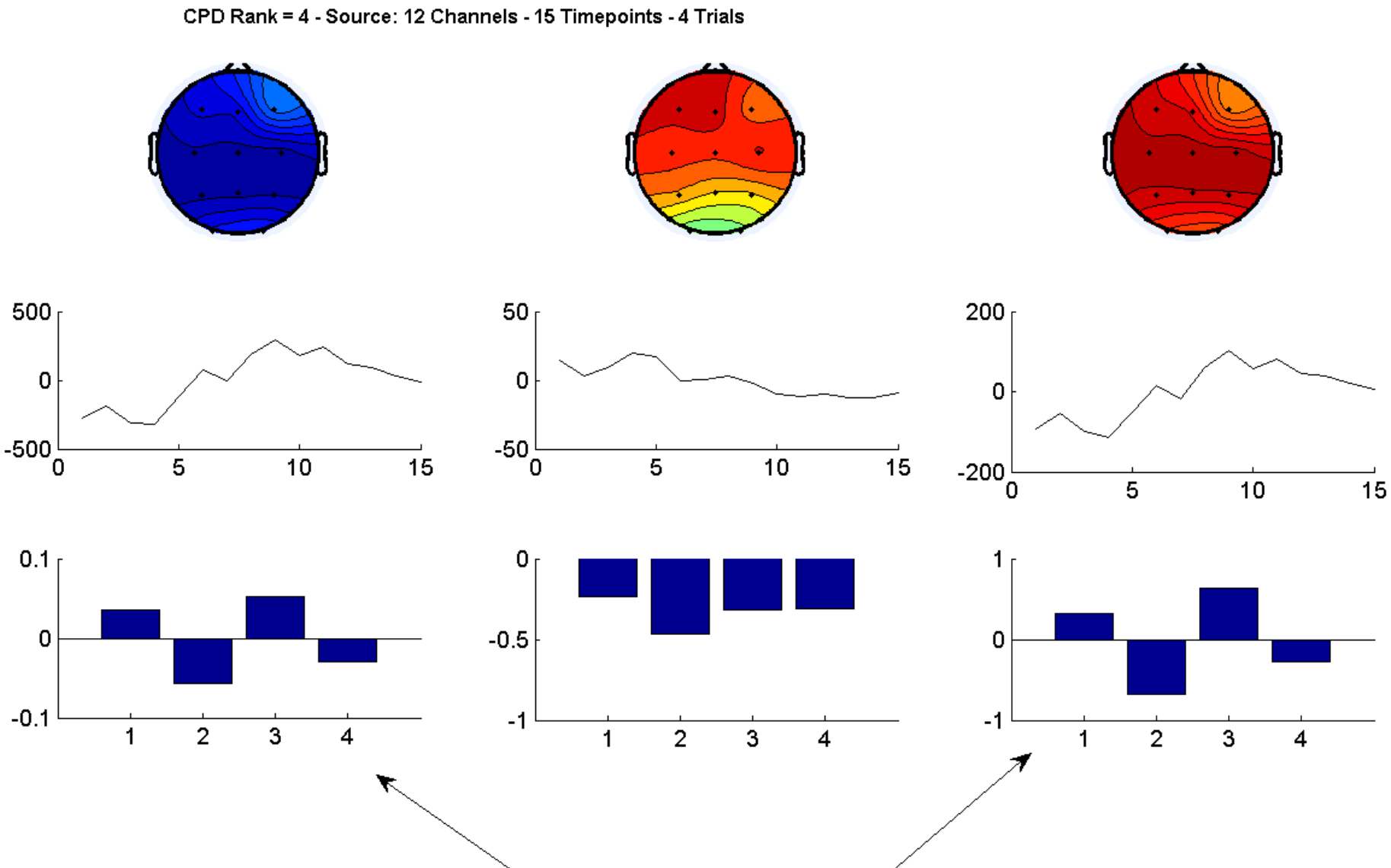
- Use knowledge

Degenerate terms



What to use?

- Algorithms
  - `cpd` if standard options
  - `cpd_nls` if non-standard options like other compression algorithm.
  - `cpd_minf` if non-standard options, and `cpd_nls` is too slow or is not accurate

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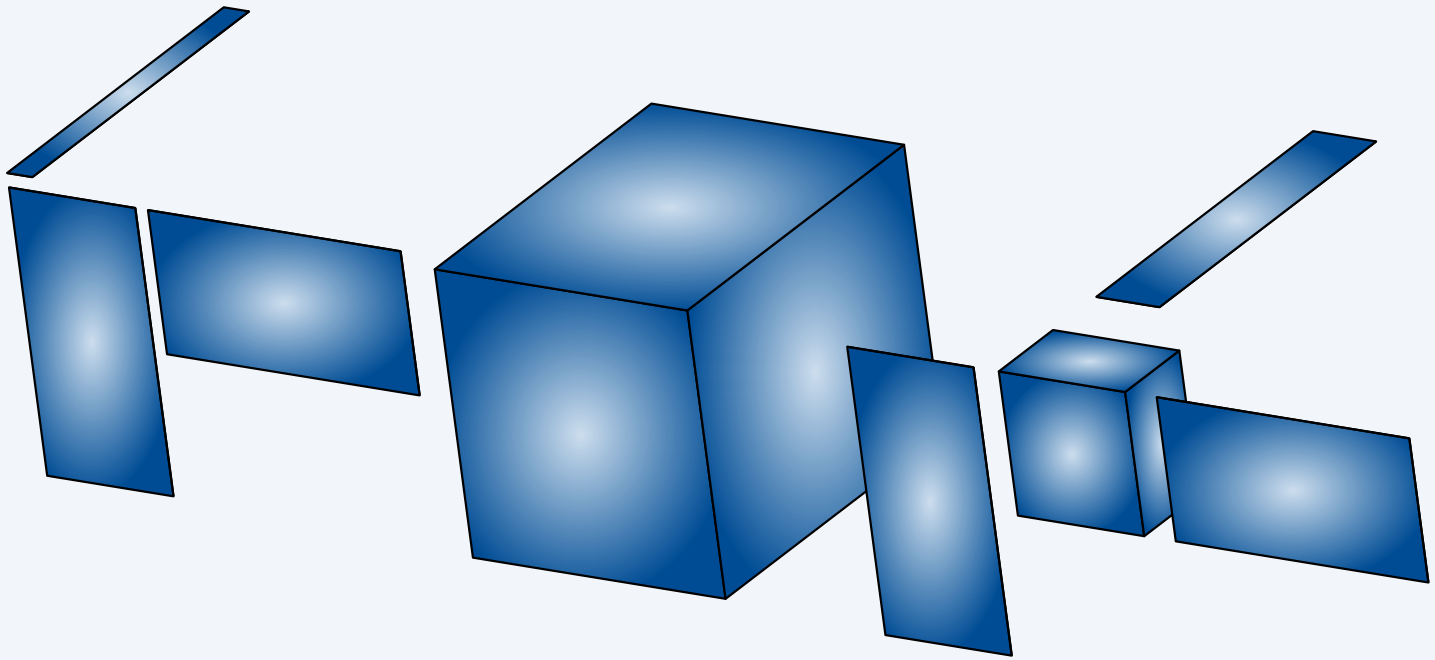
  - `cpd_nls` if non-standard options like other compression algorithm.
  - `cpd_minf` if non-standard options, and `cpd_nls` is too slow or is not accurate
- Tips
  - Try denoising
    - `mlsvd`, `lmlra_rff`
  - Multiple initializations:
    - Set `options.Initialization = @cpd_rnd` in `cpd`
    - Use `cpd_gevd` in `cpd_nls`
  - Use multistage initialization
    - compression, initialization, decomposition, refinement

Block Term Decomposition



General BTD

- Objective function

$$\min \frac{1}{2} \left\| \mathcal{T} - \sum_{r=1}^{R} \left[\!\left[\mathcal{S}^{(r)}; \mathbf{U}^{(r,1)}, \ldots, \mathbf{U}^{(r,N)} \right]\!\right] \right\|^2$$

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- Tips
  - Many initializations
  - Try denoising
  - Use a large number of iterations

Functions and algorithms

- BTD format

```
% U = { {U^(1,1), ..., U^(1,N), S^(1)}, ...,
%       {U^(R,1), ..., U^(R,N), S^(R)} }
```

Functions and algorithms

- BTD format

```
% U = { {U^(1,1), ..., U^(1,N), S^(1)}, ...,
%        {U^(R,1), ..., U^(R,N), S^(R)} }
```

- `btd_rnd`

```
U = btd_rnd([100, 100, 100], {[5,6,7], [3 2 1]});
```

Functions and algorithms

- BTD format

```
% U = { {U^(1,1), ..., U^(1,N), S^(1)}, ...,
%        {U^(R,1), ..., U^(R,N), S^(R)} }
```

- `btd_rnd`

```
U = btd_rnd([100, 100, 100], {[5,6,7], [3 2 1]});
```

- `btd_nls` and `btd_minf`

```
[U, output] = btd_nls(T, Uinit, options);
```

Block term decomposition

"... BTD is the most important decomposition in the future. I am going to work on it." – *Frederik*

$(L_r, L_r, 1)$ decomposition

- Objective function

$$\min \frac{1}{2} \left\| \mathcal{T} - \sum_{r=1}^{R} (\mathbf{A}_r \mathbf{B}_r^{\mathsf{T}}) \otimes \mathbf{c}_r \right\|^2$$

$(L_r, L_r, 1)$ decomposition

- Objective function

$$\min \frac{1}{2} \left\| \mathcal{T} - \sum_{r=1}^{R} (\mathbf{A}_r \mathbf{B}_r^{\mathsf{T}}) \otimes \mathbf{c}_r \right\|^2$$

- How to compute?
  - It is a BTD
    - `btd_nls`
  - It is a CPD (with structure)
    - `sdf_nls`
  - It is an LL1 decomposition
    - `ll1_gevd`, `ll1_nls`, `ll1_cpd`

How to compute: BTD

- Matlab

```
L = [3 3 2]
R = arrayfun(@(l) [l l 1], L, 'uni', 0);
Uinit = btd_rnd(size(T), R);

Ures = btd_nls(T, Uinit, options);
```

- Still a core tensor

How to compute: SDF

```
LL1 = @(z,state) struct_LL1(z,state,L);
size_tens = size(T)
model.variables.a = randn(size_tens(1), sum(L));
model.variables.b = randn(size_tens(2), sum(L));
model.variables.c = randn(size_tens(3), length(L));
model.factors.A = {'a'};
model.factors.B = {'b'};
model.factors.C = {'c', LL1};
model.factorizations.cpd.data = T;
model.factorizations.cpd.cpd = {'A', 'B', 'C'};

[sol, output] = sdf_nls(model, options);
uvar = struct2cell(sol.variables);
usol = struct2cell(sol.factors);

Trec = cpdgen(usol);
```

How to compute: LL1

experimental

```
Uinit = ll1_rnd(size(T), L);
Ures = ll1_nls(T, Uinit, options);
Ures = ll1_cpd(T, Uinit, options);

Trec = btdgen(Ures);
```

Discussion

	Speed	Convergence	Coding	Maturity
`btd`			🥈	🥇
`sdf`	🥈			🥇
`ll1_nls`	🥈	🥇	🥇	
`ll1_cpd`	🥇	🥈	🥇	

Tips

- Use `lll_gevd`:

```
[U, output] = lll_gevd(T, L);
```

⚠ check if `output.L = L`

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[U, output] = lll_gevd(T, L);
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Tips

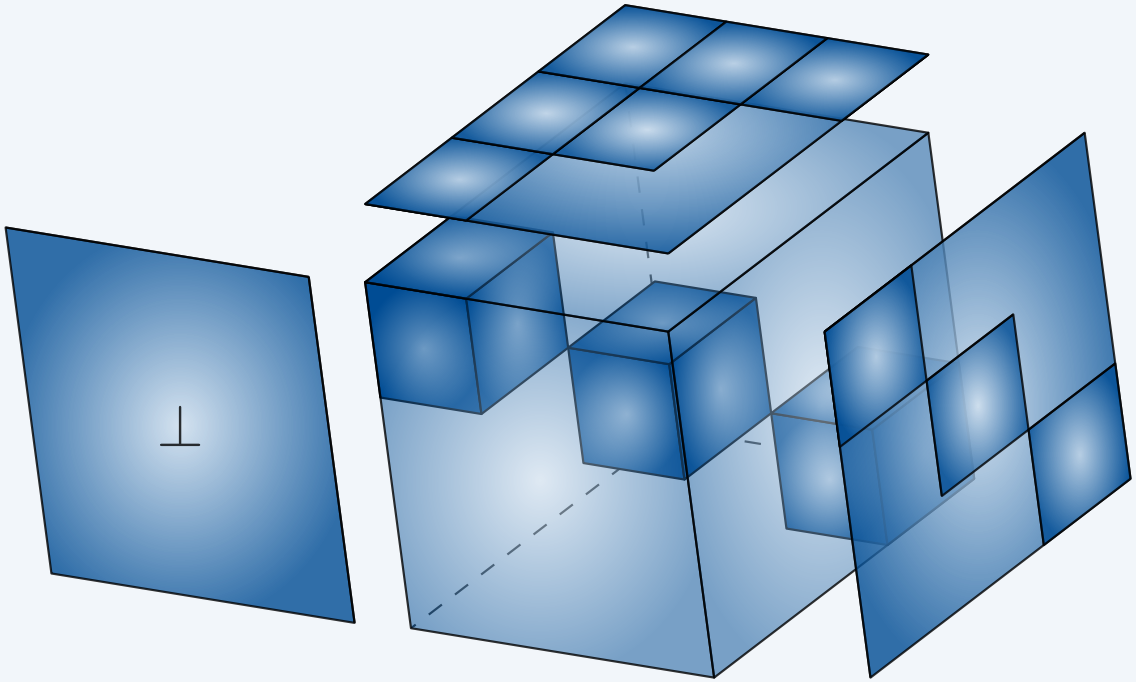
- Use `lll_gevd`:

```
[U, output] = lll_gevd(T, L);
```

⚠ check if `output.L = L`

- Use multiple initializations (not only `lll_gevd`)
- If `T` is large or noisy, compress first: `lmlra_aca`, `lmlra_rff`, `mlsvd`

Structured Data Fusion



Analysis of multiple datasets

- Suppose

$$\min_{\mathbf{x}} f(\mathbf{x}) \quad \text{with} \quad f(\mathbf{x}) = \sum_{d=1}^{D} \omega_d f^{(d)}(\mathbf{x})$$

$$f^{(d)}(\mathbf{x}) = \sum_{d=1}^{D} \frac{1}{2} \left\| \mathcal{M}^{(d)}(\mathbf{x}) - \mathcal{T}^{(d)} \right\|^2$$

in which $\mathcal{M}^{(d)}(\mathbf{x})$ is a CPD, BTD, LMLRA, ...

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$$\min_{\mathbf{x}} f(\mathbf{x}) \quad \text{with} \quad f(\mathbf{x}) = \sum_{d=1}^{D} \omega_d f^{(d)}(\mathbf{x})$$

$$f^{(d)}(\mathbf{x}) = \sum_{d=1}^{D} \frac{1}{2} \left|\left| \mathcal{M}^{(d)}(\mathbf{x}) - \mathcal{T}^{(d)} \right|\right|^2$$

  in which $\mathcal{M}^{(d)}(\mathbf{x})$ is a CPD, BTD, LMLRA, ...

- The derivative of a sum is the sum of the derivatives:

$$\nabla_{\mathbf{x}} f = \sum_{d=1}^{D} \omega_d \nabla_{\mathbf{x}} f^{(d)}$$

Implementation of constraints

- Suppose $\mathbf{x}$ is a function of $\mathbf{z}$:

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- The system of equations to compute the step becomes:

$$(\nabla_{\mathbf{z}} \mathbf{x})^{\mathsf{H}} \left(\mathbf{J}_{\mathbf{x}}^{\mathsf{H}} \mathbf{J}_{\mathbf{x}}\right) (\nabla_{\mathbf{z}} \mathbf{x}) \, \mathbf{p} = -\mathbf{g}$$

The structure of a structure

```
function [x, state] = struct_log(z, task)
if isempty(task) || (isempty(task.l) && isempty(task.r))
    % Evaluation of x(z)
    x = log(z);
    state.deriv = 1./z;
elseif ~isempty(task.r)
    % Computation of (∇_z x)*task.r, task.r = p
    x = task.deriv.*task.r;
elseif ~isempty(task.l)
    % Computation of (∇_z x)^H*state.l
    %  1. state.l = ∇_x f
    %  2. state.l = ((J_x^H J_x)(∇_z x) p)
    x = conj(task.deriv).*task.l;
end
```

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    %  2. state.l = ((J_x^H J_x)(∇_z x) p)
    x = conj(task.deriv).*task.l;
end
```

- `state.l/r` contains relevant part of factor matrix
- A little bit more complex for complex numbers

Using SDF

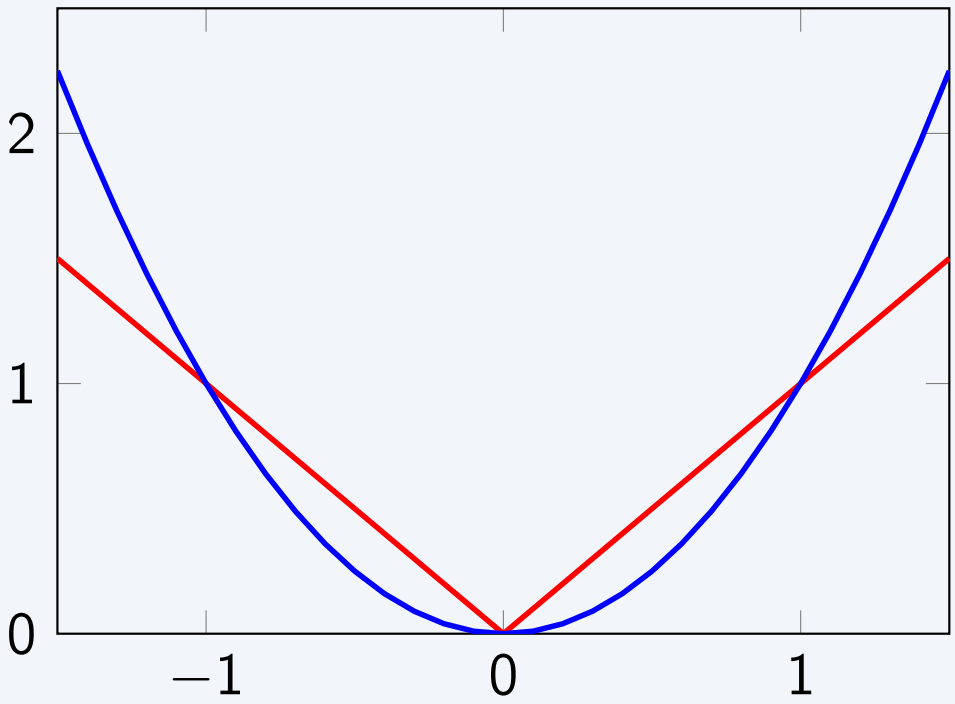
```
model.variables.a = randn(10, 5);
model.variables.b = randn(5, 5);
model.variables.c = randn(10, 1);
model.factors.A = {'a', rand(10,5)};
model.factors.B = {1, {2, @struct_nonneg}; rand(5,5)};
model.factors.B = {1, {1, @struct_nonneg}};
model.factors.C = {{'c', @struct_log, @struct_diag}};

model.factorizations.biotensor.data = T;
model.factorizations.biotensor.cpd = {'A', 'B', 'C'};

[sol, output] = sdf_nls(model, options);
uvar = struct2cell(sol.variables);
usol = struct2cell(sol.factors);
```

Regularization

```
model.factorizations.myreg.regL1 = {'A'};
model.factorizations.yourreg.regL2 = {2};
model.factorizations.yourreg.data = ones(10,10);
```



Setting options

- Similar as before

Setting options

- Similar as before
- Choice of weights $\omega_d = \frac{\bar{\omega}_d}{2\text{numel}(\mathcal{T}^{(d)})}$

```
options.RelWeights = [10 100 1];
```

Workflow for SDF

Main idea: initialize using solution of relaxed problem

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- Constraints
  1. Solve unconstrained problem
  2. Estimate parameters
  3. Add constraint and solve again

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  1. Solve problem for one dataset
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- Data fusion
  1. Solve problem for one dataset
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  3. Re-estimate fixed factors
  4. Repeat
- But only do this when no (good) direct solution can be found

Harmonic retrieval example

- Sequence of planar wave fronts measured on a $I \times J$ grid of sensors for K samples

$$t_{ijk} = \sum_{r=1}^{R} s_{kr} \mathrm{e}^{\jmath \alpha_r (i-1)} \mathrm{e}^{\jmath \beta_r (j-1)}$$

- Written as a CPD

$$\mathcal{T} = [\![\mathbf{A}, \mathbf{B}, \mathbf{S}]\!]$$

in which $\mathbf{A}$ and $\mathbf{B}$ have a Vandermonde structure

$$\mathbf{a}_r = \begin{bmatrix} 1 & \mathrm{e}^{\jmath \alpha_r} & \dots & \mathrm{e}^{\jmath \alpha_r (I-1)} \end{bmatrix}^{\mathsf{T}}$$

Harmonic retrieval: SDF

```
vandermonde = @(z, state) ...
              struct_vander(z, state, [0 sz(1)-1]);
model.variables.a = randn(1, R) + randn(1, R) * 1i;
model.variables.b = randn(1, R) + randn(1, R) * 1i;
model.variables.s = randn(sz(3), R) + randn(sz(3),R)*1i;
model.factors.A = {'a', vandermonde, @struct_transpose};
model.factors.B = {'b', vandermonde, @struct_transpose};
model.factors.S = {'s'};
model.factorizations.hr.data = Td;
model.factorizations.hr.cpd = {'A', 'B', 'S'};

[sol, output] = sdf_nls(model, options);
uvar = struct2cell(sol.variables);
usol = struct2cell(sol.factors);
```

Harmonic retrieval: SDF

```
        fval                relfval            relstep
        =1/2*norm(F)^2      TolFun = 1e-08     TolX = 1e-08

   0:   3.36998907e+04 |
   1:   3.33852257e+03 | 9.00933727e-01 | 3.000000e-01
  20:   1.38581644e+00 | 5.16779039e-07 | 1.637907e-02
  40:   1.27729165e+00 | 5.00268067e-08 | 8.947791e-03
  60:   1.25247376e+00 | 1.92818795e-08 | 3.601389e-03
  80:   1.23919216e+00 | 1.58284013e-08 | 3.639052e-03
 100:   1.23055086e+00 | 1.08583537e-08 | 2.393667e-03
 104:   1.22912806e+00 | 9.92786005e-09 | 2.178808e-03

err =
    0.8311    0.7563    0.5319
```

Harmonic retrieval: CPD + SDF

```
Uinit = cpd_rnd(Td, R, struct('Imag', @randn));
Ures = cpd_nls(Td, Uinit, options);

alpha_est = mean(Ures{1}(2:end,:)./Ures{1}(1:end-1,:));
beta_est = mean(Ures{2}(2:end,:)./Ures{2}(1:end-1,:));
S_est = Ures{3};

model.variables.a = alpha_est;
model.variables.b = beta_est;
model.variables.s = S_est;
```

Harmonic retrieval: CPD + SDF

```
        fval                relfval            relstep
        =1/2*norm(F)^2      TolFun = 1e-08     TolX = 1e-08

   0:   1.33180211e+03 |
   1:   1.30137568e+03 | 2.28460581e-02 | 3.000000e-01
  12:   9.42652003e-10 | 1.79934766e-10 | 8.970192e-05

err = [0.6386    0.6573    0.0000]

   0:   2.53718572e+00 |
   7:   7.60910370e-11 | 2.74361409e-09 | 1.175042e-04

err = 1.0e-05 * [0.1585    0.1230    0.2147]
```

Non-negativity constraints: SDF

```
Uinit = cpd_rnd(Tn, R, 'real', @rand, 'orth', false);

model.variables = cellfun(@(u) sqrt(u), Uinit, 'uni', 0);
model.factors.A = {1, @struct_nonneg};
model.factors.B = {2, @struct_nonneg};
model.factors.C = {3, @struct_nonneg};
model.factorizations.cpd.data = Tn;
model.factorizations.cpd.cpd = {'A', 'B', 'C'};

[sol, output] = sdf_nls(model);
Usdf = struct2cell(sol.factors);
```

Non-negativity constraints: CPD

```
LB = cellfun(@(u) zeros(size(u)), Uinit, 'uni', 0);
UB = cellfun(@(u) inf(size(u)), Uinit, 'uni', 0);

options = struct;
options.Algorithm = @(F,dF,z0,options) ...
    nlsb_gndl(F, dF, LB, UB, z0, options);

[Ures, output] = cpd_nls(Tn, Uinit, options);
```

Non-negativity constraints

A little experiment:

- $\mathbf{A}, \mathbf{B}, \mathbf{C} \in \mathcal{U}(0,1)^{200\times 10}$
- $\mathcal{T} = [\![\mathbf{A}, \mathbf{B}, \mathbf{C}]\!]$ with rank 10

	`sdf`	`nlsb`	`nls`
Iterations	73	30	11
Time (s)	5.75	1.80	0.70
Time/it (ms)	79	60	63

Tips and tricks

- Use solutions to relaxed problems as initialization
- Be aware of alternatives if speed is important

Random remarks

- Be careful when using `tic` and `toc`

```
timer = tic; cpd(...); toc(timer)
```

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timer = tic; cpd(...); toc(timer)
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- Use `noisy`, `cpdgen`, `cpderr`, ...

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timer = tic; cpd(...); toc(timer)
```

- Use `noisy`, `cpdgen`, `cpderr`, ...
- Master `cellfun`

```
U = cellfun(@(u) u(:,1), U, 'uni', 0);
```

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timer = tic; cpd(...); toc(timer)
```

- Use `noisy`, `cpdgen`, `cpderr`, ...
- Master `cellfun`

```
U = cellfun(@(u) u(:,1), U, 'uni', 0);
```

- Get the development version from git
  - Register at bitbucket.org
  - Send username to me
  - Clone tensorlab

Workflow

1. Be lazy
2. Try other parameters
3. Try other initialization techniques
4. Try other algorithms