A Two-phase Framework with a Bézier Simplex-based Interpolation Method for Computationally Expensive Multi-objective Optimization

GECCO 2022 at Boston

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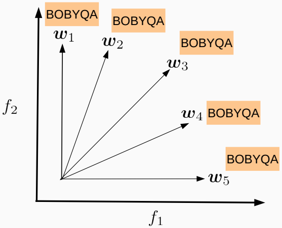
Four-phased HMO-CMA-ES [Loshchilov 16] performs well for expensive opt.

1st phase runs BOBYQA on K scalar optimization problems

- BOBYQA [Powell 09]: SOTA mathematical derivative-free optimizer
  - It iteratively solves a trust region sub-problem using quadratic models



- 1st phase uses only the $10 \times N$ fevals *in total* (N = Num. variables)
- 2nd: SS-MO-CMA-ES → 3rd: MO-CMA-ES → 4th: CMA-ES
  - HMO-CMA-ES shows an excellent anytime performance ☺

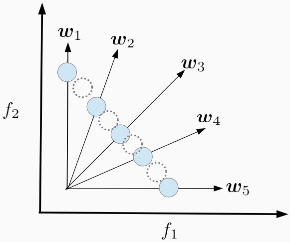
Ilya Loshchilov, Tobias Glasmachers: Anytime Bi-Objective Optimization with a Hybrid Multi-Objective CMA-ES (HMO-CMA-ES). GECCO (Companion) 2016: 1169-1176

M. J. D. Powell. 2009. The BOBYQA algorithm for bound constrained optimization without derivatives. Technical Report DAMTP 2009/NA06. University of Cambridge

One drawback of the 1st phase in HMO-CMA-ES

It can achieve only K sparsely distributed solutions

- Only a limited number of fevals are available
- K needs to be as small as possible ($K = 5$ in ↙)



Motivation

- Can this issue be addressed by a solution interpolation approach?

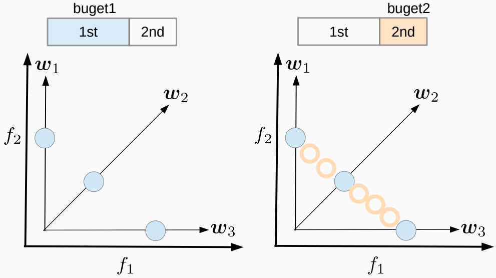
Proposed: A Two-Phase framework with a Bézier simplex-based interpolation method (TPB)

1st phase is similar to that in HMO-CMA-ES

- It runs BOBYQA on K scalar problems, but its details are different
  - K = Num. objectives $+1$ $(= 2 + 1 = 3$ in this study)
  - The normalization procedure, a budget allocation strategy, the order of scalar optimization, control parameters of BOBYQA, etc.

2nd phase interpolates the $K(= 3)$ solutions by the Bézier simplex

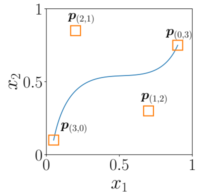
- It is theoretically well-founded and can fit the K solutions



Bézier simplex: A generalized version of the Bézier curve to higher dims

The Bézier curve

$(M = 2,\ N = 2,\ D = 3)$



The Bézier simplex

$(M = 3,\ N = 3,\ D = 3)$

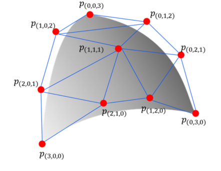


Figure 2: A Bézier simplex for $M = 3$, $D = 3$.

From [Kobayashi 19]

- M: Num. objectives, N: Num. variables, D: Degree of a model
  - D determines the number of control points $\boldsymbol{p}_{\boldsymbol{d}_1}, \ldots \in \mathbb{R}^N$
  - Control points define a Bézier simplex model
- It can describe the Pareto optimal solution set $\boldsymbol{X}^\star$ [Kobayashi 19]
  - When $\boldsymbol{X}^\star$ is homeomorphic to an $(M-1)$-dim. simplex [Hamada 20]
  - The theoretically well-founded nice property for the interpolation ☺

Ken Kobayashi, Naoki Hamada, Akiyoshi Sannai, Akinori Tanaka, Kenichi Bannai, Masashi Sugiyama: Bézier Simplex Fitting: Describing Pareto Fronts of Simplicial Problems with Small Samples in Multi-Objective Optimization. AAAI 2019: 2304-2313

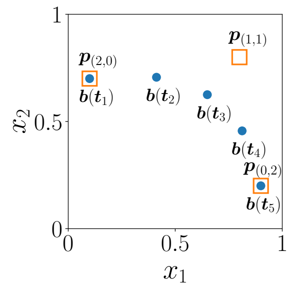
Naoki Hamada, Kenta Hayano, Shunsuke Ichiki, Yutaro Kabata, Hiroshi Teramoto: Topology of Pareto Sets of Strongly Convex Problems. SIAM J. Optim. 30(3): 2659-2686 (2020)

Example: Bézier simplex with $M = 2$ (N. obj), $N = 2$ (N. var), and $D = 2$

A Bézier simplex model $\boldsymbol{b} : \boldsymbol{t} \mapsto \boldsymbol{b}(\boldsymbol{t})$

$$\boldsymbol{b}(\boldsymbol{t}) = t_1^2 \boldsymbol{p}_{(2,0)} + 2 t_1 t_2 \boldsymbol{p}_{(1,1)} + t_2^2 \boldsymbol{p}_{(0,2)}$$

- Input $\boldsymbol{t} \in \mathbb{R}^M$: a parameter vector, and $\sum_{m=1}^{M} t_m = 1, t_m \geq 0$
- Output $\boldsymbol{b}(\boldsymbol{t}) \in \mathbb{R}^N$: a mapping of $\boldsymbol{t}$. It can be a solution $\boldsymbol{x} \in \mathbb{R}^N$
- Model parameters $\boldsymbol{p}_{\boldsymbol{d}_1}, \ldots \in \mathbb{R}^N$: Control points



- $\boldsymbol{p}_{(2,0)} = (0.1, 0.7)$
- $\boldsymbol{p}_{(1,1)} = (0.8, 0.8)$
- $\boldsymbol{p}_{(0,2)} = (0.9, 0.2)$
- $\boldsymbol{t}_1 = (1, 0) \mapsto \boldsymbol{b}(\boldsymbol{t}_1) = (0.1, 0.7)$
- $\boldsymbol{t}_2 = (0.75, 0.25) \mapsto \boldsymbol{b}(\boldsymbol{t}_2) \approx (0.41, 0.71)$
- $\boldsymbol{t}_3 = (0.5, 0.5) \mapsto \boldsymbol{b}(\boldsymbol{t}_3) \approx (0.65, 0.63)$
- $\boldsymbol{t}_4 = (0.25, 0.75) \mapsto \boldsymbol{b}(\boldsymbol{t}_4) \approx (0.81, 0.46)$
- $\boldsymbol{t}_5 = (0, 1) \mapsto \boldsymbol{b}(\boldsymbol{t}_5) = (0.9, 0.2)$

Bézier simplex fitting to approximate a solution set X [Kobayashi 19]

- Let $\boldsymbol{X} = \{\boldsymbol{x}_k \in \mathbb{R}^N\}_{k=1}^K$ be a solution set of size K
- Let $\boldsymbol{T} = \{\boldsymbol{t}_k \in \Delta^{M-1} \subseteq \mathbb{R}^M\}_{k=1}^K$ be a parameter vec. set of size K
  - $\boldsymbol{t}_k$ corresponds to $\boldsymbol{x}_k$
- We want a Bézier simplex model $\boldsymbol{b}$ that approximates $\boldsymbol{X}$
  - How do we set control points, e.g., $\boldsymbol{p}_{(2,0)}$, $\boldsymbol{p}_{(1,1)}$, and $\boldsymbol{p}_{(0,2)}$?
- The Bézier simplex fitting method adjusts the control points ($\boldsymbol{p}_{\boldsymbol{d}}$) by minimizing the ordinary least squares loss function:

$$\text{minimize} \quad \sum_{k=1}^{K} \|\boldsymbol{x}_k - \boldsymbol{b}(\boldsymbol{t}_k)\|^2$$

- The loss function is a convex quadratic function with respect to $\boldsymbol{p}_{\boldsymbol{d}}$
- Its minimizer can be found by solving a normal equation

The PyTorch implementation is available at

`https://github.com/rafcc/pytorch-bsf`

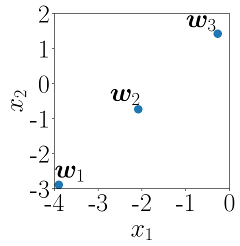
Ken Kobayashi, Naoki Hamada, Akiyoshi Sannai, Akinori Tanaka, Kenichi Bannai, Masashi Sugiyama: Bézier Simplex Fitting: Describing Pareto Fronts of Simplicial Problems with Small Samples in Multi-Objective Optimization. AAAI 2019: 2304-2313

1st phase applies BOBYQA to K scalar optimization problems $\{g_{\boldsymbol{w}_k}\}_{k=1}^{K}$

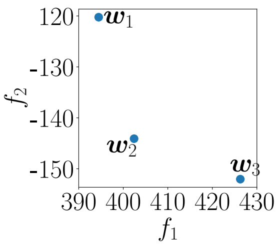
- We set $K = 2 + 1 = 3$, $\boldsymbol{w}_1 = (0, 1)$, $\boldsymbol{w}_2 = (0.5, 0.5)$, $\boldsymbol{w}_1 = (1, 0)$
  - K should be $K \geq M + 1$ to handle the nonlinear PS set
- We use the weighted sum function as in HMO-CMA-ES
  - TPB can use any g, e.g., the weighted Tchebycheff function
- We set a budget ratio $r^{\text{1st}} = 0.9$
  - e.g., $\texttt{budget}^{\text{1st}} = 0.9 \times 40 = 36$ fevals when $\texttt{budget} = 40$ fevals
  - Each run of BOBYQA can use $\texttt{budget}^{\text{1st}}/K = 36/3 = 12$ fevals

Results on f_1 (Sphere/Sphere) with $N = 2$ in `bbob-biobj`

Solution space



Objective space



2nd phase interpolates the K sol. by a Bézier simplex model-based method

2.1 The fitting phase

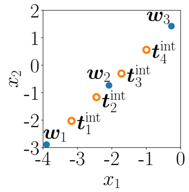
- The 1st phase obtained $\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3\}$ using $\boldsymbol{W} = \{\boldsymbol{w}_1, \boldsymbol{w}_2, \boldsymbol{w}_3\}$
- TPB treats $\boldsymbol{w}_k$ as $\boldsymbol{t}_k^{\text{fit}}$, and $\boldsymbol{T}^{\text{fit}} = \{\boldsymbol{t}_1, \boldsymbol{t}_2, \boldsymbol{t}_3\}$
- TPB fits a Bézier simplex model $\boldsymbol{b}$ to $\boldsymbol{X}$ with $\boldsymbol{T}^{\text{fit}} = \boldsymbol{W}$

2.2 The solution generation phase

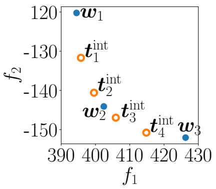
- $\texttt{budget}^{\text{2nd}} = \texttt{budget} - \texttt{budget}^{\text{1st}} = 40 - 36 = 4$ in this example
- 4 solutions are generated by giving $\boldsymbol{t}_1^{\text{int}}, \boldsymbol{t}_2^{\text{int}}, \boldsymbol{t}_3^{\text{int}}, \boldsymbol{t}_4^{\text{int}}$ to $\boldsymbol{b}$
  - We equally generate parameters on Δ^{M-1}, removing $(0, 1)$ and $(1, 0)$

Results on f_1 (D-Sphere) with $N = 2$ in `bbob-biobj`

Solution space



Objective space



- $\boldsymbol{t}_1^{\text{int}} = (0.2, 0.8)$
- $\boldsymbol{t}_2^{\text{int}} = (0.4, 0.6)$
- $\boldsymbol{t}_3^{\text{int}} = (0.6, 0.4)$
- $\boldsymbol{t}_4^{\text{int}} = (0.8, 0.2)$

Advantages and disadvantages of TPB

Advantages ☺

1. TPB can use any SOTA single-objective black-box optimizer
2. TPB can exploit the structure of the PS set
3. TPB is faster than model-based optimizers, e.g., ParEGO [Knowles 06]

Disadvantages ☹

1. The poor anytime performance as in most two-phase approaches
   - They can obtain only a poor-quality solution set when they stop before reaching the maximum budget [Dubois-Lacoste 11]
   - But, this is true for most model-based optimizers (due to the LHS)
2. It performs poorly when the PS topology cannot be a simplex
   - The $15/55$ unimodal `bbob-biobj` problems would be OK
   - The $40/55$ multimodal `bbob-biobj` problems would be NG

Joshua D. Knowles: ParEGO: a hybrid algorithm with on-line landscape approximation for expensive multiobjective optimization problems. IEEE Trans. Evol. Comput. 10(1): 50-66 (2006)

Jérémie Dubois-Lacoste, Manuel López-Ibáñez, Thomas Stützle: Improving the anytime behavior of two-phase local search. Ann. Math. Artif. Intell. 61(2): 125-154 (2011)

Experimental setup

- All experiments were conducted using COCO [Hansen 21]
    - The 55 `bbob-biobj` problems [Brockhoff 22] with $N \in \{2, 3, 5, 10, 20\}$
    - I_{COCO}: The uncrowded HV based on the unbounded external arch.
        - When none of objective points dominates the reference point $\boldsymbol{z}$, I_{COCO} is based on the smallest distance to the ROI defined by $\boldsymbol{z}$
- We compare TPB with HMO-CMA-ES [Loshchilov 16] and ...
    - ParEGO [Knowles 06], MOTPE [Ozaki 20], K-RVEA [Chugh 18], KTA2 [Song 21], and EDN-ARMOEA [Guo 22]
    - Maximum fevals: $20 \times N$, $30 \times N$, and $40 \times N$
- Parameter setting for TPB:
    - The number of weight vectors K in the 1st phase: 3
    - The budget ratio in the 1st phase r^{1st}: 0.9
    - The degree of a Bézier simplex D: 2

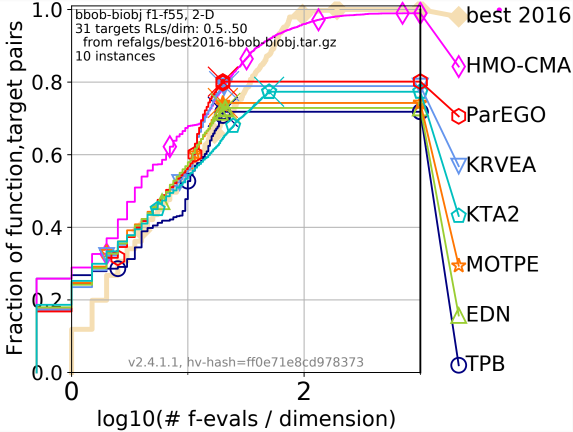
Nikolaus Hansen, Anne Auger, Raymond Ros, Olaf Mersmann, Tea Tušar, Dimo Brockhoff: COCO: a platform for comparing continuous optimizers in a black-box setting. Optim. Methods Softw. 36(1): 114-144 (2021)

Dimo Brockhoff, Anne Auger, Nikolaus Hansen, Tea Tušar: Using Well-Understood Single-Objective Functions in Multiobjective Black-Box Optimization Test Suites. Evol. Comput. 30(2): 165-193 (2022)

Results on the 55 bbob-biobj problems with $N = 2$ (max. fevals $= 40$)

HMO-CMA-ES shows the best anytime performance

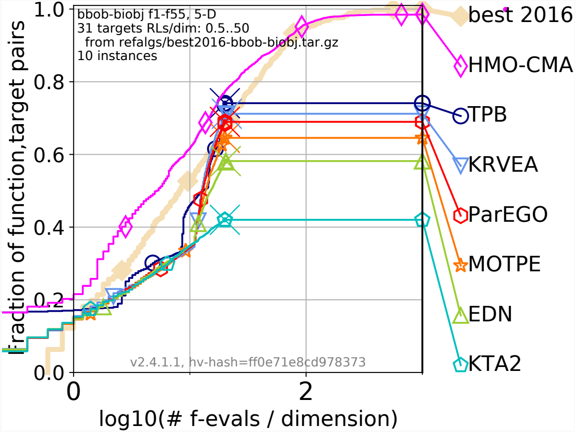
- ParEGO is the best optimizer at $20 \times N$ fevals
- TPB is the second-worst optimizer



Results on the 55 bbob-biobj problems with $N = 5$ (max. fevals $= 100$)

TPB performs better than the five model-based optimizers

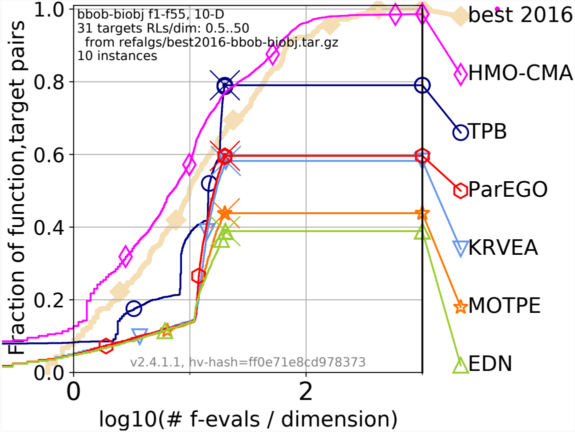
- HMO-CMA-ES performs the best



Results on the 55 `bbob-biobj` problems with $N = 10$ (max. fevals $= 200$)

TPB performs better than HMO-CMA-ES at $20 \times N$ fevals

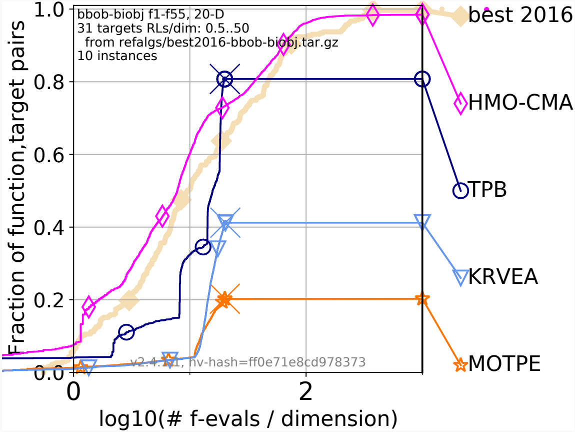
- TPB outperforms the model-based optimizers at anytime
- Because KTA2 was too time-consuming, it was removed



Results on the 55 `bbob-biobj` problems with $N = 20$ (max. fevals $= 400$)

TPB performs better than HMO-CMA-ES at $20 \times N$ fevals

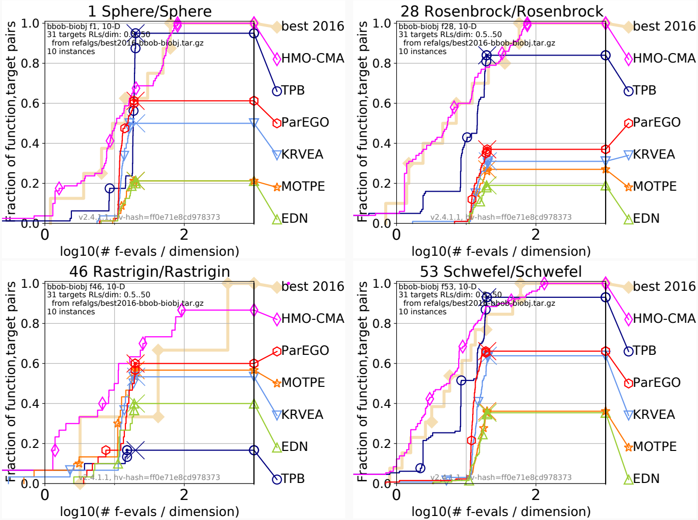
- Because ParEGO and EDN were time-consuming, they were removed



Results on f_1, f_{28}, f_{46}, f_{53} with $N = 10$ (max. fevals = 200)

We did not expect the results on f_{53} with no simplex structure

- The Bézier simplex can represent only a standard simplex



Conclusion

Proposed: A Two-Phase framework with a Bézier simplex-based interpolation method (TPB)

- The 1st phase runs BOBYQA on K scalar optimization problems
- The 2nd phase interpolates the K solutions by the Bézier simplex
  - It can describe the PS set under under certain conditions
- The performance of TPB was investigates on `bbob-biobj`
  - TPB performs better than HMO-CMA-ES for $N \geq 10$ at max. fevals
  - TPB performs better than the five model-based optimizers for $N \geq 5$
  - TPB is computatoinally cheaper than the five optimizers

TPB can give a new perspective for expensive MO optimization

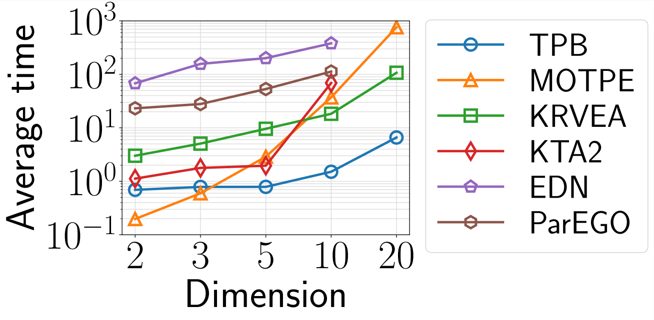
- A non-Bayesian optimization approach
- The use of the Bézier simplex for MO optimization

Future work

- An extension of TPB to optimization with more than 2 objectives
- An extension of TPB to initialize the population in EMO

Average computation time of the optimizers over the 15 instances of f_1

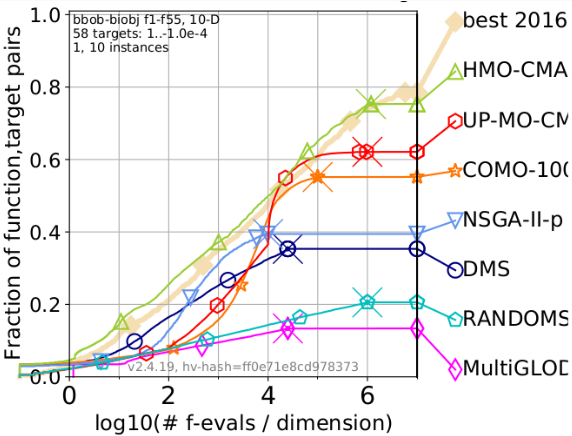
- TPB is the fastest for $N \geq 5$
- Meta-model-based optimizers are generally time-consuming
  - Especially for a larger N



Comparison of 7 optimizers on `bbob-biobj` for N. var $N = 10$ [Brockhoff 21]

HMO-CMA-ES performs the best for $10^2 \times N$ (= $1\,000$) fevals

- HMO-CMA-ES performs well for computationally expensive opt.



Dimo Brockhoff, Baptiste Plaquevent-Jourdain, Anne Auger, Nikolaus Hansen: DMS and MultiGLODS: black-box optimization benchmarking of two direct search methods on the bbob-biobj test suite. GECCO Companion 2021: 1251-1258

Definition of the Bézier simplex (M: Num. obj, N: Num. var, D: Degree)

The standard $(M-1)$-simplex

$$\Delta^{M-1} = \left\{ \boldsymbol{t} = (t_1, \dots, t_M) \in \mathbb{R}^M \middle| \sum_{m=1}^{M} t_m = 1,\ t_m \geq 0 \right\}$$

- E.g., $\boldsymbol{t} = (0.2, 0.8)$ and $\boldsymbol{t} = (1, 0)$ for $M = 2$

A set of non-negative integers

$$\mathbb{N}_D^M := \left\{ \boldsymbol{d} = (d_1, \dots, d_M) \in \mathbb{N}^M \middle| \sum_{m=1}^{M} d_m = D \right\}$$

- E.g., $\mathbb{N}_2^2 = \{\boldsymbol{d} = (d_1, d_2) \in \mathbb{N}^2 | d_1 + d_2 = 2\} = \{(2,0), (1,1), (0,2)\}$

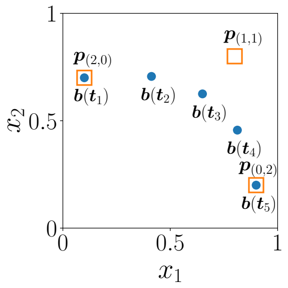
A Bézier simplex, $\boldsymbol{b} : \Delta^{M-1} \to \mathbb{R}^N$, $\boldsymbol{b} : \boldsymbol{t} \mapsto \boldsymbol{b}(\boldsymbol{t})$

$$\boldsymbol{b}(\boldsymbol{t}) = \sum_{\boldsymbol{d} \in \mathbb{N}_D^M} \binom{D}{\boldsymbol{d}} \boldsymbol{t}^{\boldsymbol{d}} \boldsymbol{p}_{\boldsymbol{d}}$$

- $\boldsymbol{p}_{\boldsymbol{d}} \in \mathbb{R}^N$ is a control point, e.g., $\boldsymbol{p}_{(2,0)} = (4.1, -3.2)$, $\boldsymbol{p}_{(1,1)} = (2.6, 0)$
- $\binom{D}{\boldsymbol{d}} := \frac{D!}{d_1! \dots d_M!}$ is a multinomial coefficient, e.g., $\binom{2}{(2,0)}$
- $\boldsymbol{t}^{\boldsymbol{d}} := t_1^{d_1} \dots t_M^{d_M}$ is a monomial for each $\boldsymbol{t}$ and $\boldsymbol{d}$, e.g., $\boldsymbol{t}^{(2,0)} = (t_1^2, t_2^0)$

Example: Bézier simplex with $M = 2$ (N. obj), $N = 2$ (N. var), and $D = 2$

$$
\begin{aligned}
\underline{\boldsymbol{b}(\boldsymbol{t})} &= \sum_{\boldsymbol{d} \in \mathbb{N}_D^M} \binom{D}{\boldsymbol{d}} \boldsymbol{t}^{\boldsymbol{d}} \boldsymbol{p}_{\boldsymbol{d}}, \\
&= \binom{2}{(2,0)} t_1^2 t_2^0 \boldsymbol{p}_{(2,0)} + \binom{2}{(1,1)} t_1^1 t_2^1 \boldsymbol{p}_{(1,1)} + \binom{2}{(0,2)} t_1^0 t_2^2 \boldsymbol{p}_{(0,2)} \\
&= \underline{t_1^2 \boldsymbol{p}_{(2,0)} + 2 t_1 t_2 \boldsymbol{p}_{(1,1)} + t_2^2 \boldsymbol{p}_{(0,2)}}
\end{aligned}
$$



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