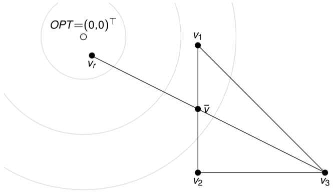
Optimization in Machine Learning

Nelder-Mead method



Learning goals

- General idea
- Reflection, expansion, contraction
- Advantages & disadvantages
- Examples

NELDER-MEAD METHOD

- Derivative-free method $\Rightarrow$ heuristic
- Generalization of bisection in d-dimensional space
- Based on d-simplex, defined by $d + 1$ points:
  - $d = 1$ interval
  - $d = 2$ triangle
  - $d = 3$ tetrahedron
  - $\cdots$

NELDER-MEAD METHOD / 2

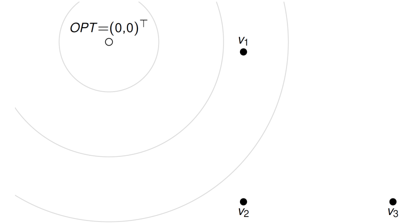
A version of the **Nelder-Mead** method:

Initialization: Choose $d + 1$ random, affinely independent points $\mathbf{v}_i$ ($\mathbf{v}_i$ are vertices: corner points of the simplex/polytope).

1. **Order**: Order points according to ascending function values

$$f(\mathbf{v}_1) \leq f(\mathbf{v}_2) \leq \ldots \leq f(\mathbf{v}_d) \leq f(\mathbf{v}_{d+1}).$$

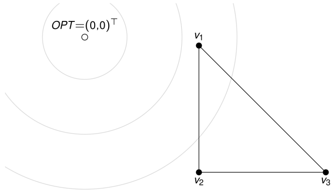
with $\mathbf{v}_1$ best point, $\mathbf{v}_{d+1}$ worst point.

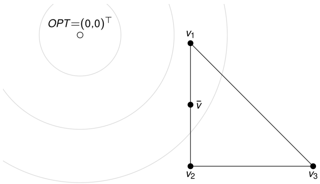


NELDER-MEAD METHOD / 3

❷ Compute **centroid** without worst point

$$\bar{\mathbf{v}} = \frac{1}{d}\sum_{i=1}^{d}\mathbf{v}_i.$$



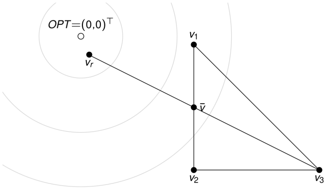


NELDER-MEAD METHOD / 4

3. **Reflection:** Compute reflection point

$$\mathbf{v}_r = \bar{\mathbf{v}} + \rho(\bar{\mathbf{v}} - \mathbf{v}_{d+1}),$$

with $\rho > 0$. Compute $f(\mathbf{v}_r)$.



Note: Default value for reflection coefficient: $\rho = 1$

NELDER-MEAD METHOD / 5

Distinguish three cases:

- **Case 1:** $f(\mathbf{v}_1) \leq f(\mathbf{v}_r) < f(\mathbf{v}_d)$

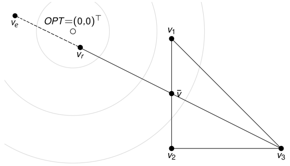
  $\Rightarrow$ Accept $\mathbf{v}_r$ and discard $\mathbf{v}_{d+1}$

- **Case 2:** $f(\mathbf{v}_r) < f(\mathbf{v}_1)$

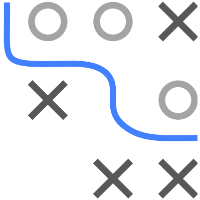
  $\Rightarrow$ **Expansion:**

$$\mathbf{v}_e = \bar{\mathbf{v}} + \chi(\mathbf{v}_r - \bar{\mathbf{v}}), \quad \chi > 1.$$

  We discard $\mathbf{v}_{d+1}$ and except the better of $\mathbf{v}_r$ and $\mathbf{v}_e$.



Note: Default value for expansion coefficient: $\chi = 2$



NELDER-MEAD METHOD / 6

- **Case 3:** $f(\mathbf{v}_r) \geq f(\mathbf{v}_d)$

  $\Rightarrow$ **Contraction:**

  $$\mathbf{v}_c = \bar{\mathbf{v}} + \gamma(\mathbf{v}_{d+1} - \bar{\mathbf{v}})$$

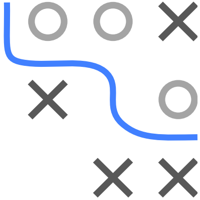
  with $0 < \gamma \leq 1/2$.

  - If $f(\mathbf{v}_c) < f(\mathbf{v}_{d+1})$, accept $\mathbf{v}_c$.
  - Otherwise, shrink **entire** simplex (**Shrinking**):

  $$\mathbf{v}_i = \mathbf{v}_1 + \sigma(\mathbf{v}_i - \mathbf{v}_1) \quad \forall i$$

  Note: Default values for contraction and shrinking coefficient:
  $\gamma = \sigma = 1/2$

4. **Repeat** all steps until stopping criterion met.



NELDER-MEAD

Advantages:

- No gradients needed
- Robust, often works well for non-differentiable functions.

Drawbacks:

- Relatively slow (not applicable in high dimensions)
- Not each step improves solution, only mean of corner values is reduced.
- No guarantee for convergence to local optimum / stationary point.

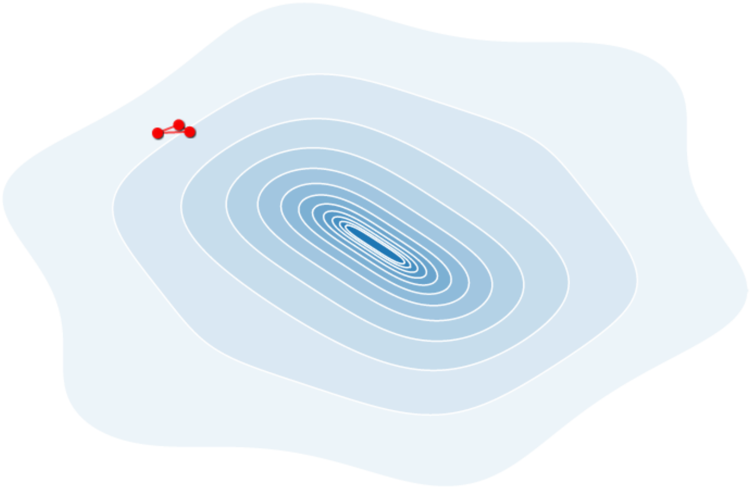
Visualization:

`http://www.benfrederickson.com/numerical-optimization/`

Note: Nelder-Mead is default method of `R` function `optim()`. If gradient is available and cheap, L-BFGS is preferred.

NELDER-MEAD VISUALIZATION IN 2D

$$\min_{\mathbf{x}} f(x_1, x_2) = x_1^2 + x_2^2 + x_1 \cdot \sin x_2 + x_2 \cdot \sin x_1$$



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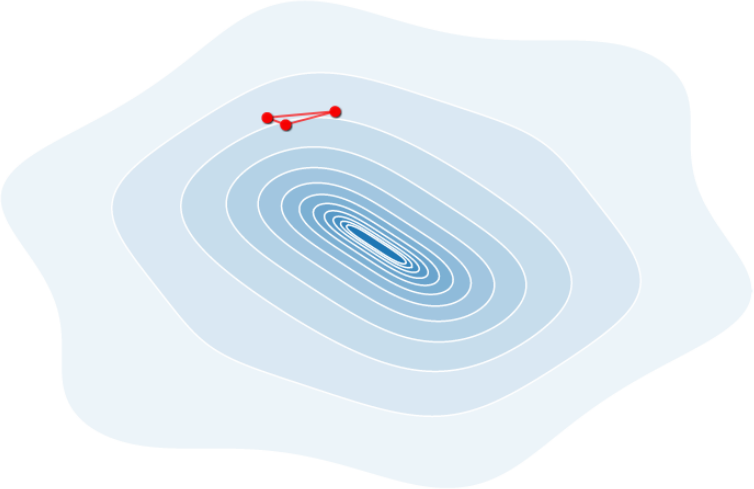

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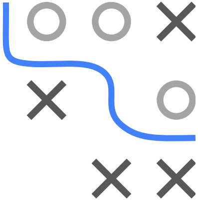

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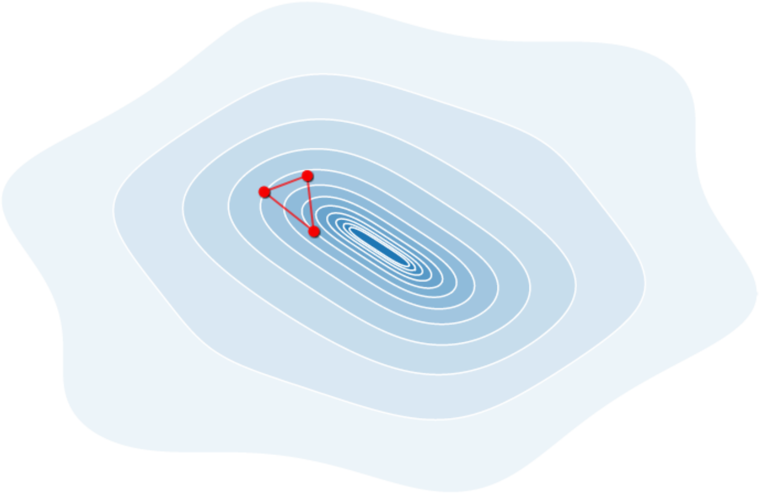

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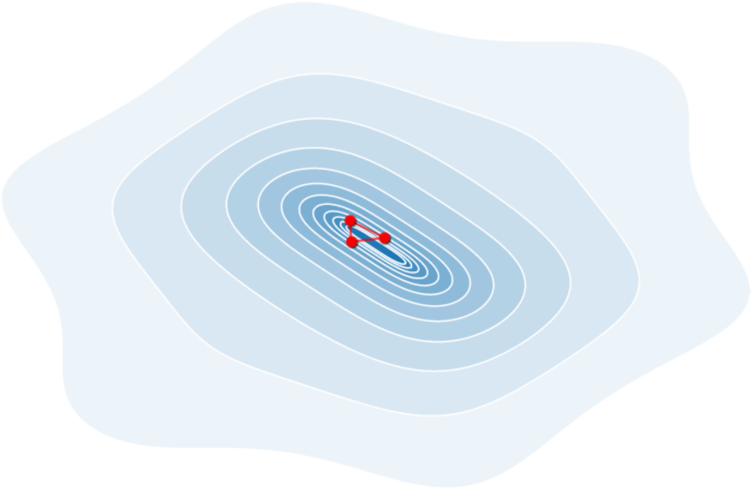
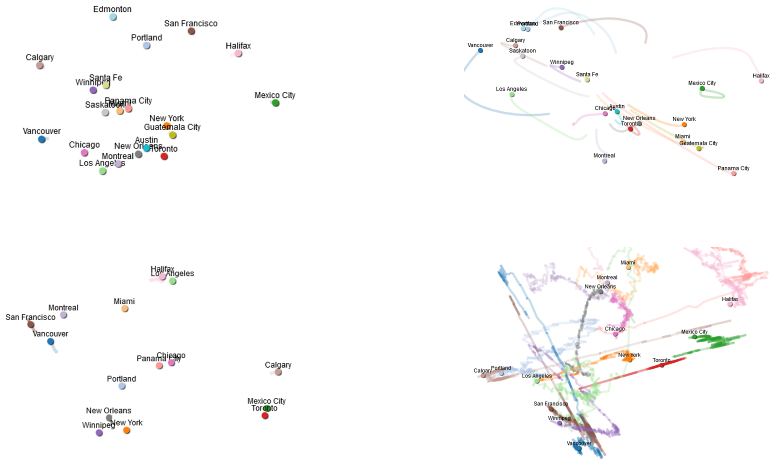
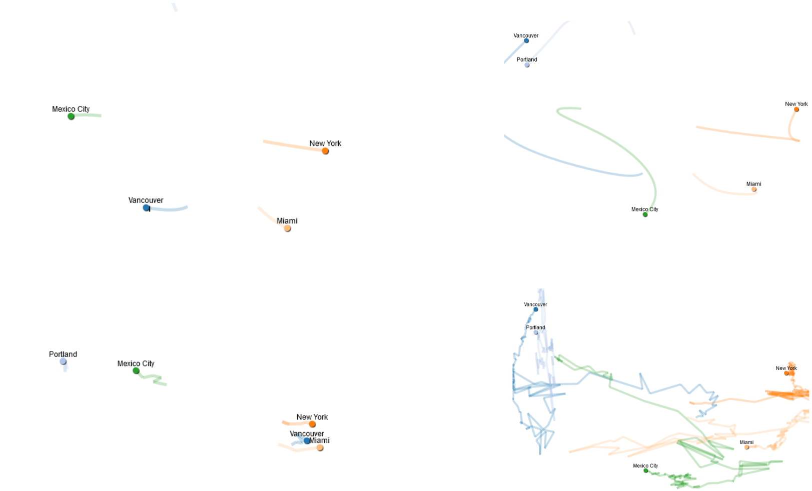


NELDER-MEAD VS. GD



Nelder-Mead in multiple dimensions: Organize points (US cities) to keep predefined mutual distances. For 10 cities, gradient descent (top) converges well for a suitable learning rate. Nelder-Mead (bottom) fails to converge, even after many iterations.

NELDER-MEAD VS. GD / 2



Even for only 5 cities, Nelder-Mead (bottom) performs poorly. However, gradient descent (top) still works.