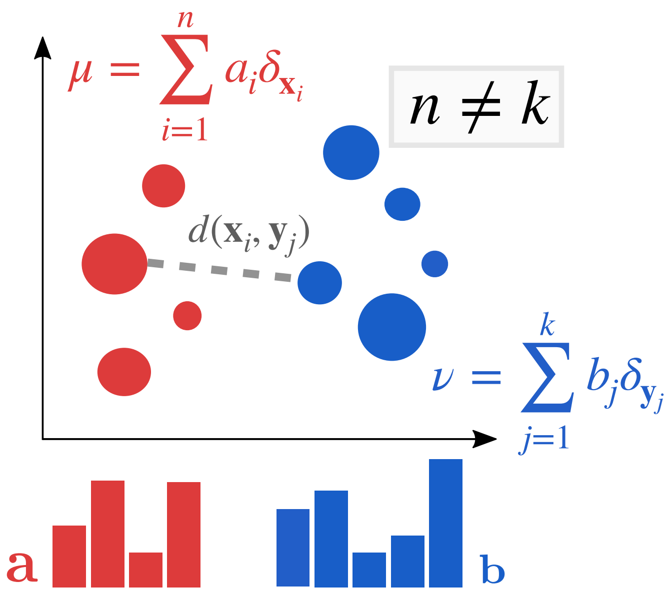
From Wasserstein to Sinkhorn

✦ Classical optimal transport (in a nutshell)



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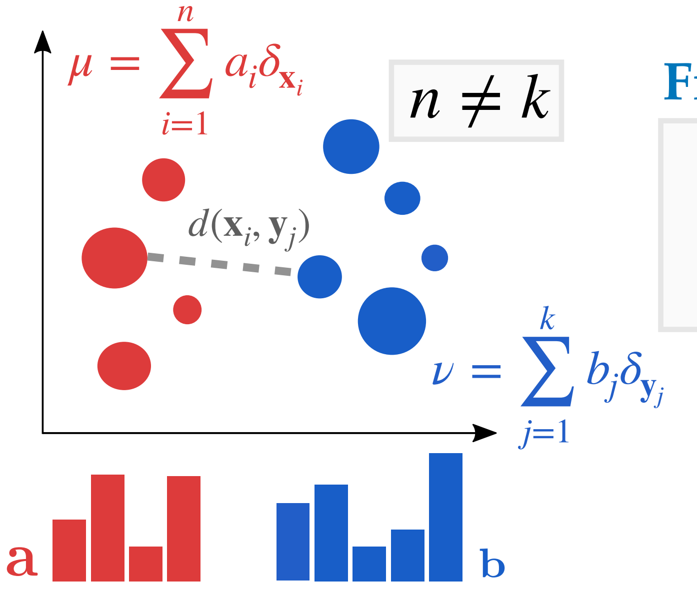

Find plan $T \in \mathbb{R}_+^{n \times k}$

$$\min_T \sum_{ij} d(\mathbf{x}_i, \mathbf{y}_j) T_{ij}$$

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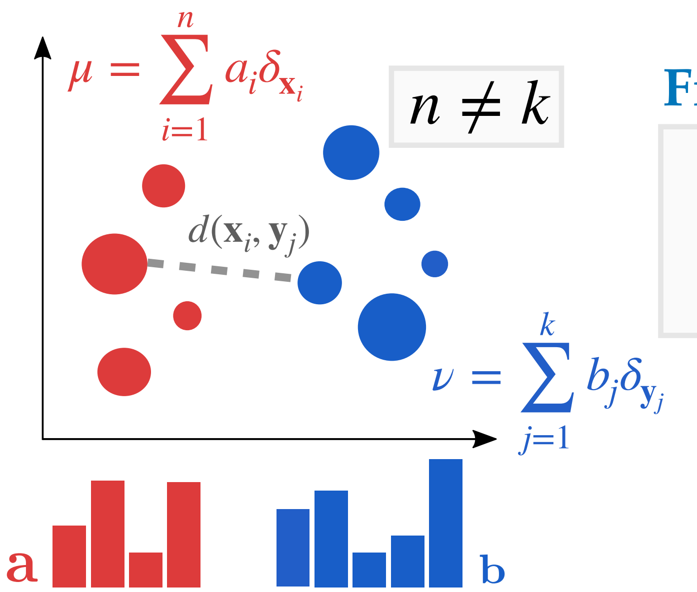

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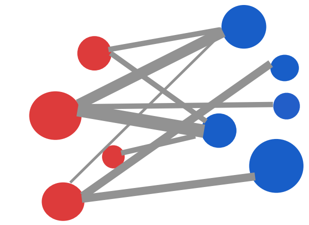
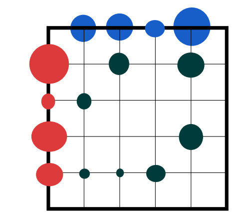
which constraints ?

Coupling $\Pi(a, b)$

$$T 1_k = a$$

$$T^\top 1_n = b$$





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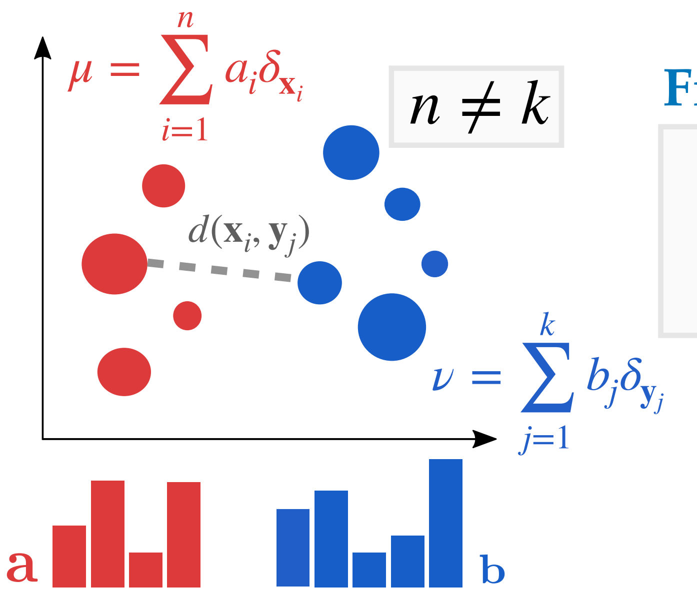

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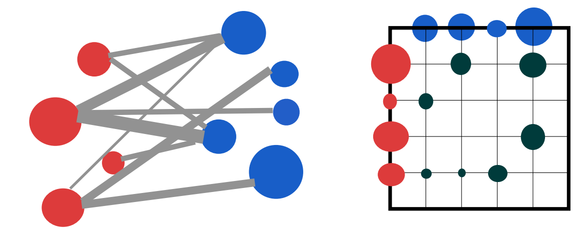

$T \in [0,1]^{n \times k}$

✦ Wasserstein distance

$\mu \in \mathscr{P}(X)$

$\nu \in \mathscr{P}(X)$

$$\mathrm{W}_p(\mu, \nu) = \left(\min_T \int_{X \times X} d(x, y)^p \; \mathrm{d}T(x, y) \right)^{1/p}$$

- It is always **well-defined**
- It is a proper distance on $\mathscr{P}(X)$
- Lifts the geometry of $X \to \mathscr{P}(X)$

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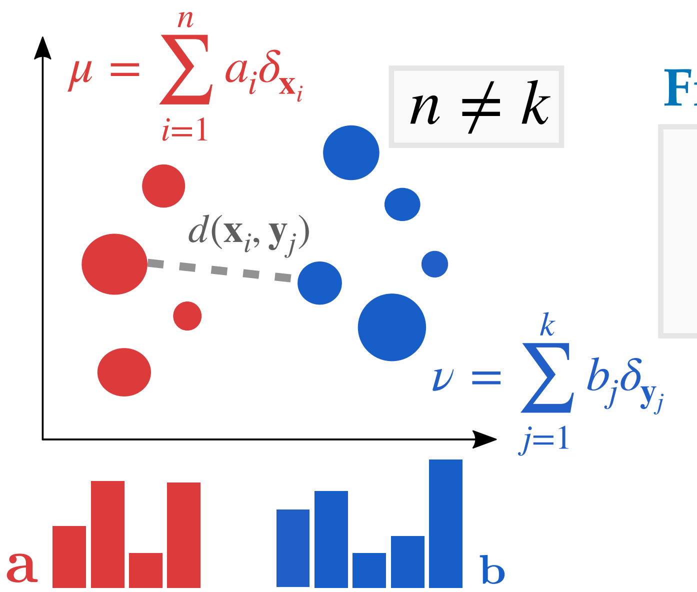

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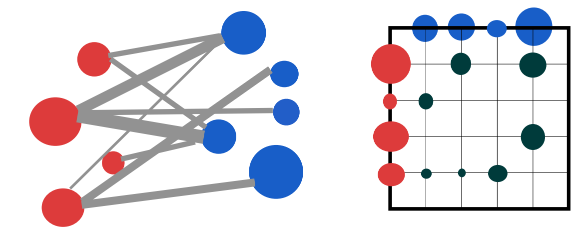

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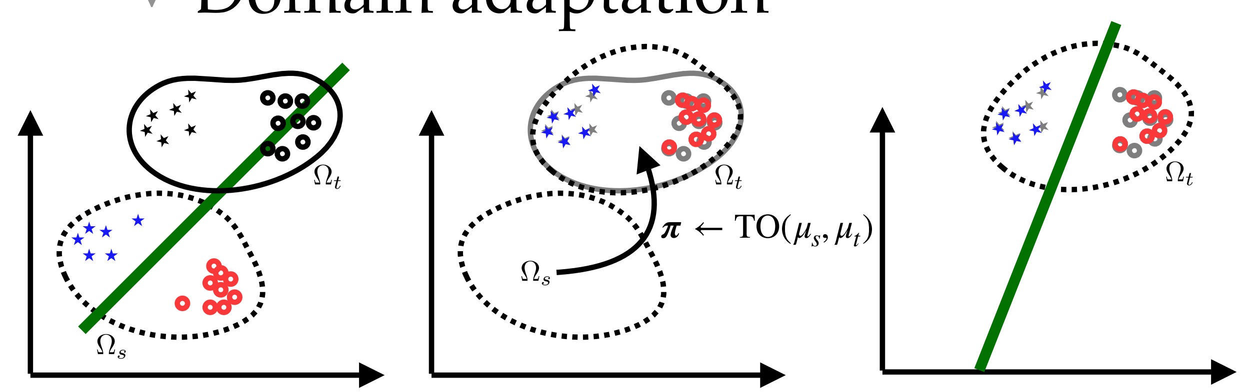
✦ In machine learning

- Domain adaptation



- Generative modeling
- Analysis of NN convergence
- ML on graphs, fairness
- And many other …

From Wasserstein to Sinkhorn

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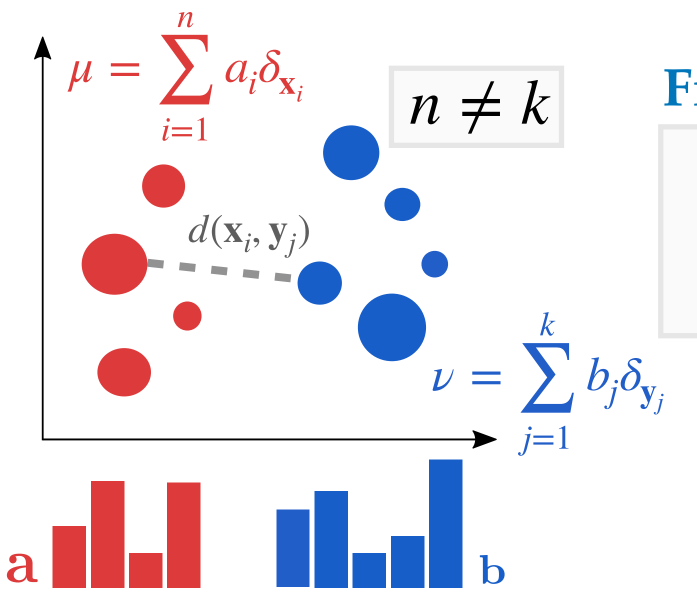

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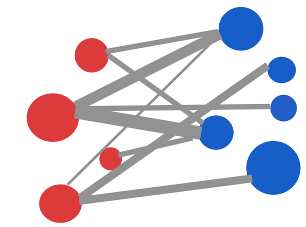

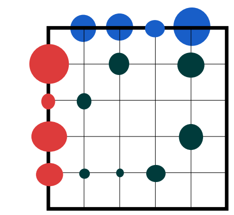

$T \in [0,1]^{n \times k}$

✦ Algorithmic fundations

Unregularized problem

✦ Simplex, Network flow

$$\mathcal{O}(n^3 \log(n)^2)$$

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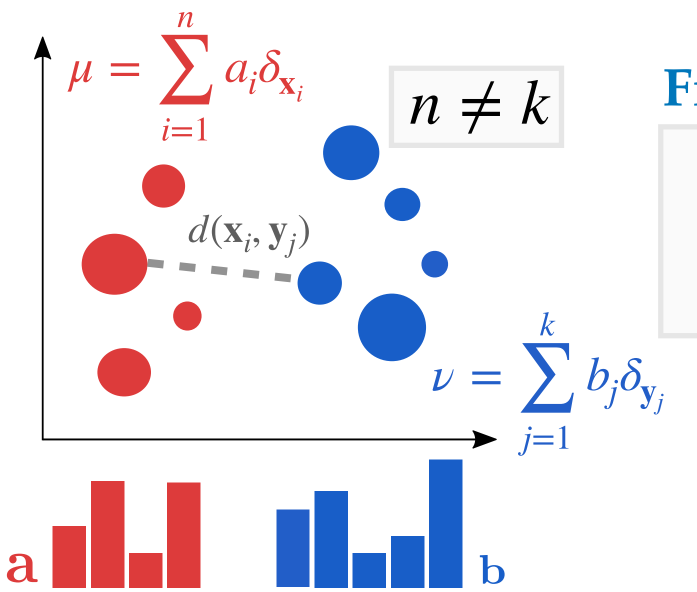

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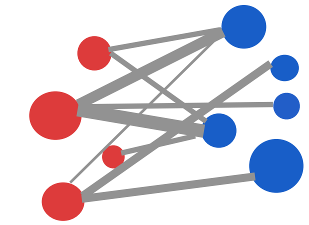

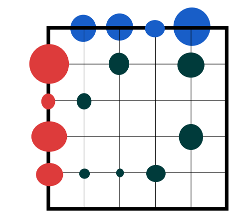

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$$\mathcal{O}(n^3 \log(n)^2)$$

Entropic regularization

$$\min_T \sum_{ij} d(\mathbf{x}_i, \mathbf{y}_j) T_{ij} - \varepsilon H(T)$$

Sinkhorn algorithm

$$K := \left(e^{-d(\mathbf{x}_i, \mathbf{y}_j)/\varepsilon}\right)_{ij}$$

```
while not converged:
```

$$u = a \oslash K^\top v$$
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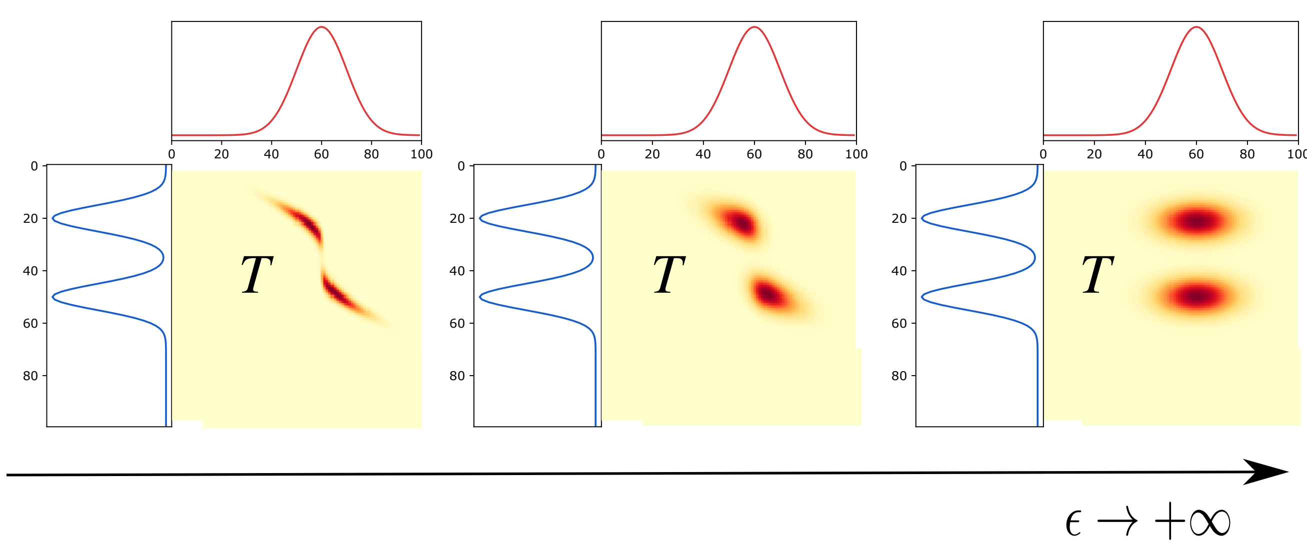
```
output
```

$$T = \mathrm{diag}(u) K \,\mathrm{diag}(v)$$



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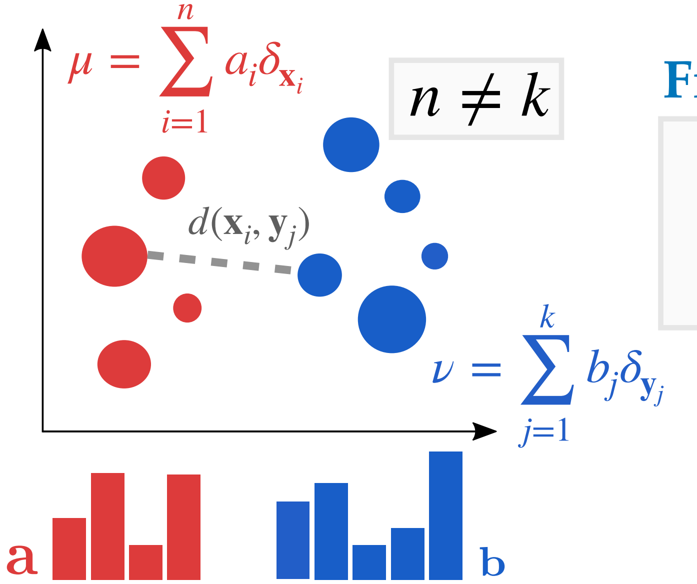

$\mu = \sum_{i=1}^{n} a_i \delta_{\mathbf{x}_i}$

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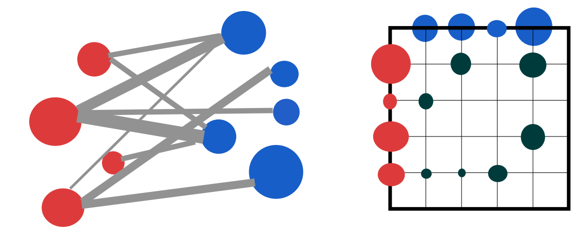

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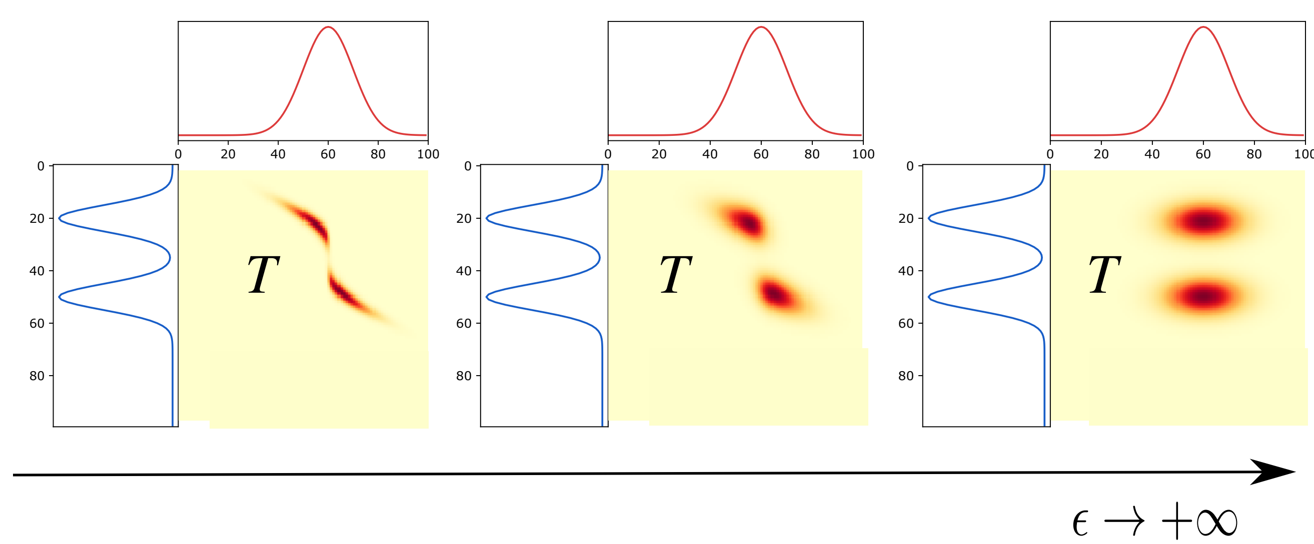

Accelerating Sinkhorn algorithm

✦ **Goal: fast approximation of** $u \to Ku$

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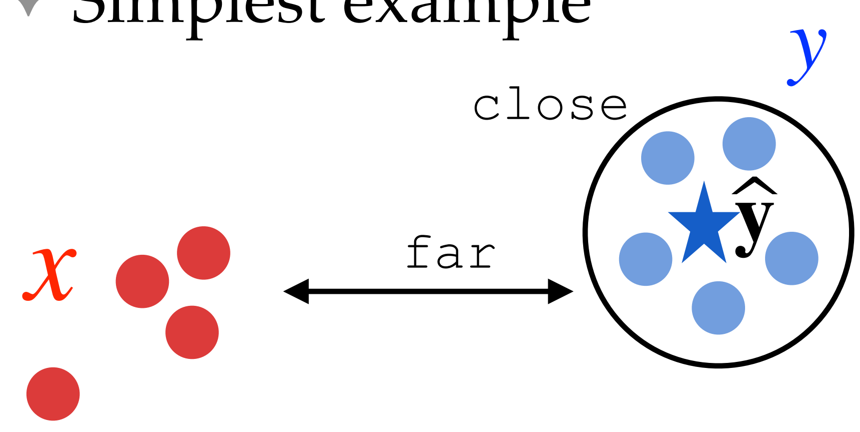

$$K \approx \mathbf{p}\mathbf{q}^\top = \begin{pmatrix} k(\mathbf{x}_1, \hat{\mathbf{y}}) \\ k(\mathbf{x}_2, \hat{\mathbf{y}}) \\ \vdots \\ k(\mathbf{x}_n, \hat{\mathbf{y}}) \end{pmatrix} 1^\top$$

$$u \to \tilde{K}u \text{ in } \mathcal{O}(n)$$

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✦ Generally if r clusters in y far enough from all the x

$$K \approx \mathbf{P}\mathbf{Q}^\top \quad u \to \tilde{K}u \text{ in } \mathcal{O}(rn)$$

✦ But unknown clusters + crude approximation !

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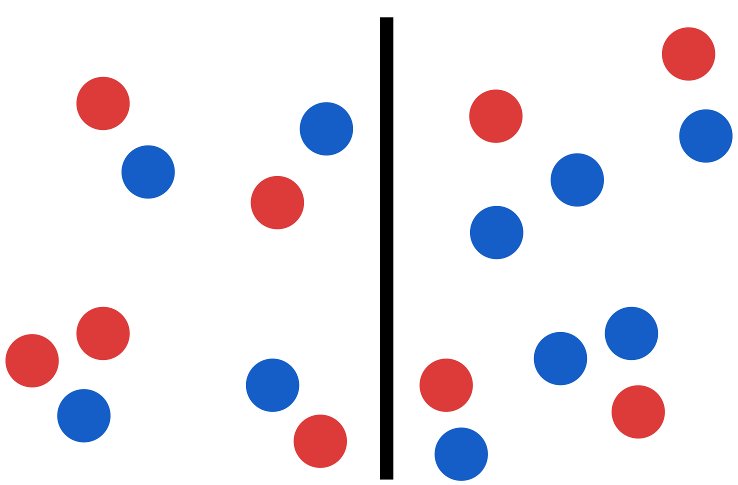

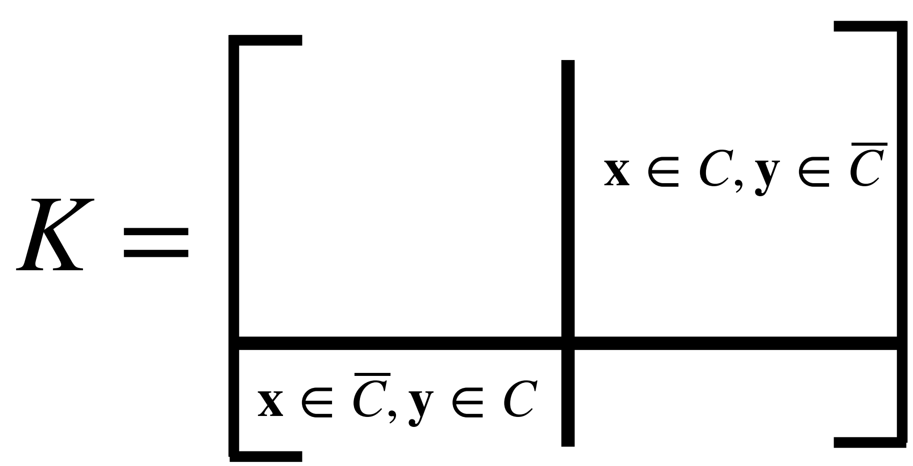

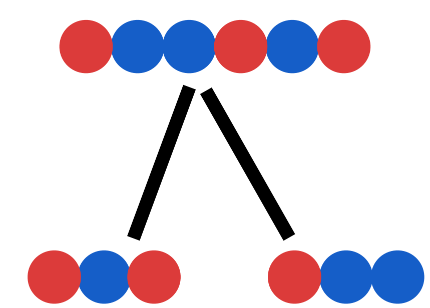

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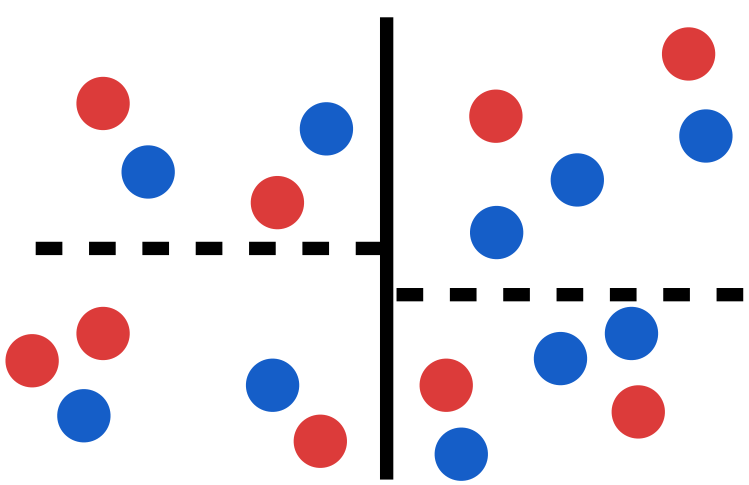

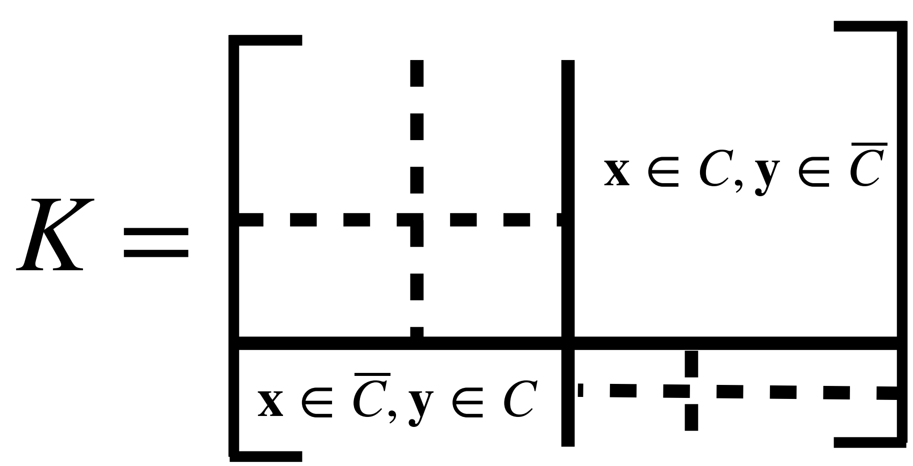

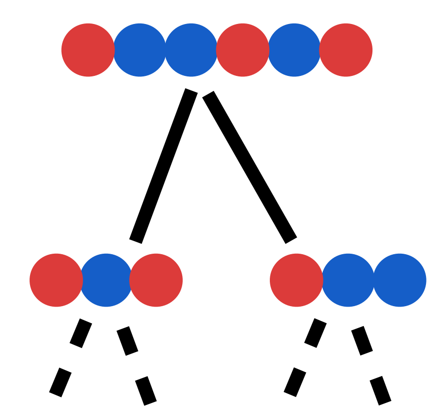

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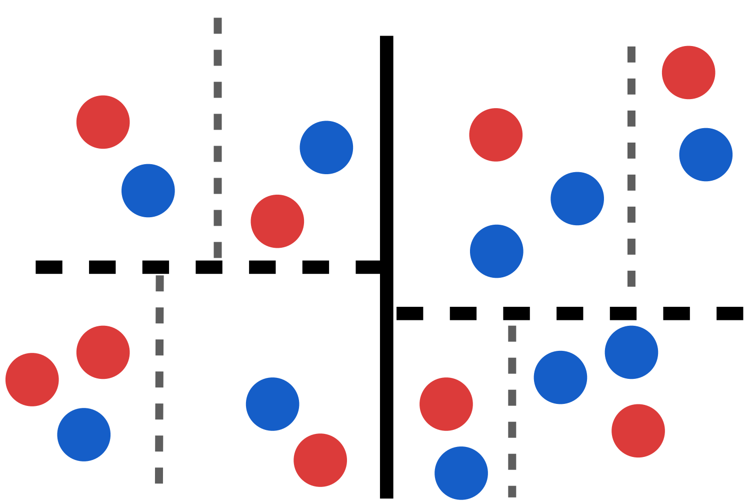
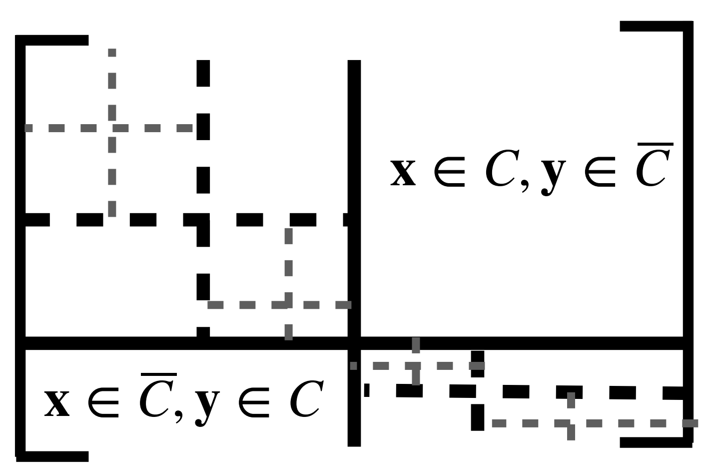
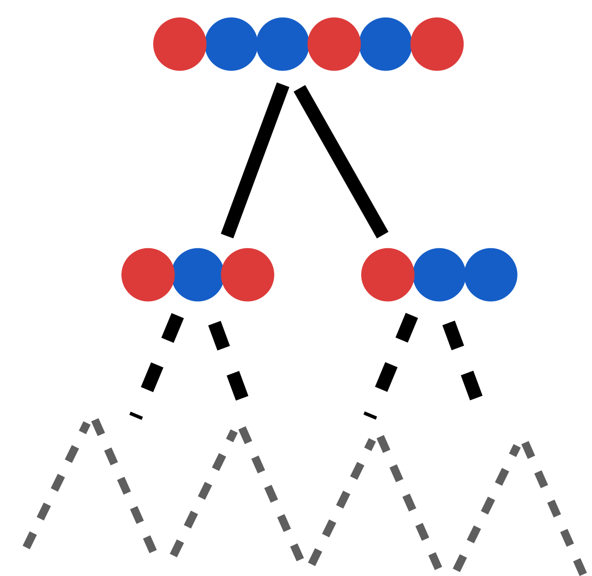


$K =$





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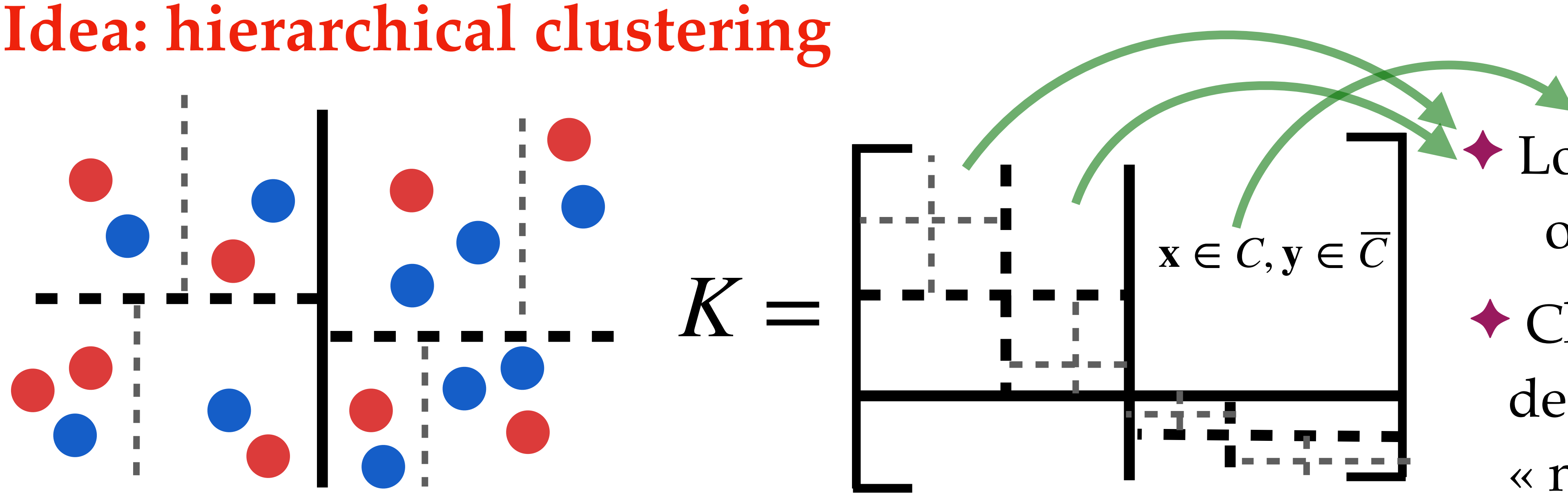

✦ Low-rank approx of « far interactions »

✦ Cheap tree traversal to detect « far » and « near » interactions

✦ Fast multipole methods, Barnes-Hut algorithm, H-matrices