Randomized Kaczmarz Algorithms: Exact MSE Analysis and Optimal Sampling Probabilities

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Large Linear Systems

$$\underbrace{\boldsymbol{y}}_{\text{observation}} = \underbrace{\boldsymbol{A}}_{\text{system matrix}} \times \boldsymbol{x} + \underbrace{\boldsymbol{z}}_{\text{noise}}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_m \end{bmatrix} = \begin{bmatrix} -\boldsymbol{a_1}^T- \\ -\boldsymbol{a_2}^T- \\ \cdot \\ \cdot \\ \cdot \\ -\boldsymbol{a_m}^T- \end{bmatrix} \times \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_n \end{bmatrix} + \begin{bmatrix} z_1 \\ z_2 \\ \cdot \\ \cdot \\ \cdot \\ z_m \end{bmatrix}$$

observation

system matrix

noise

Large Linear Systems

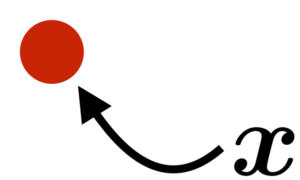
$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{bmatrix} = \begin{bmatrix} -\boldsymbol{a_1}^T- \\ -\boldsymbol{a_2}^T- \\ \vdots \\ -\boldsymbol{a_m}^T- \end{bmatrix} \times \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} + \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_m \end{bmatrix}$$

New considerations:

- Massive sizes
- Streaming data
- Distributed storage
- Parallel computing platform

$\Longrightarrow$ *Iterative greedy methods*

- Noiseless case: $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ encodes a system of m equations.



Kaczmarz Algorithm — Iterative Projections

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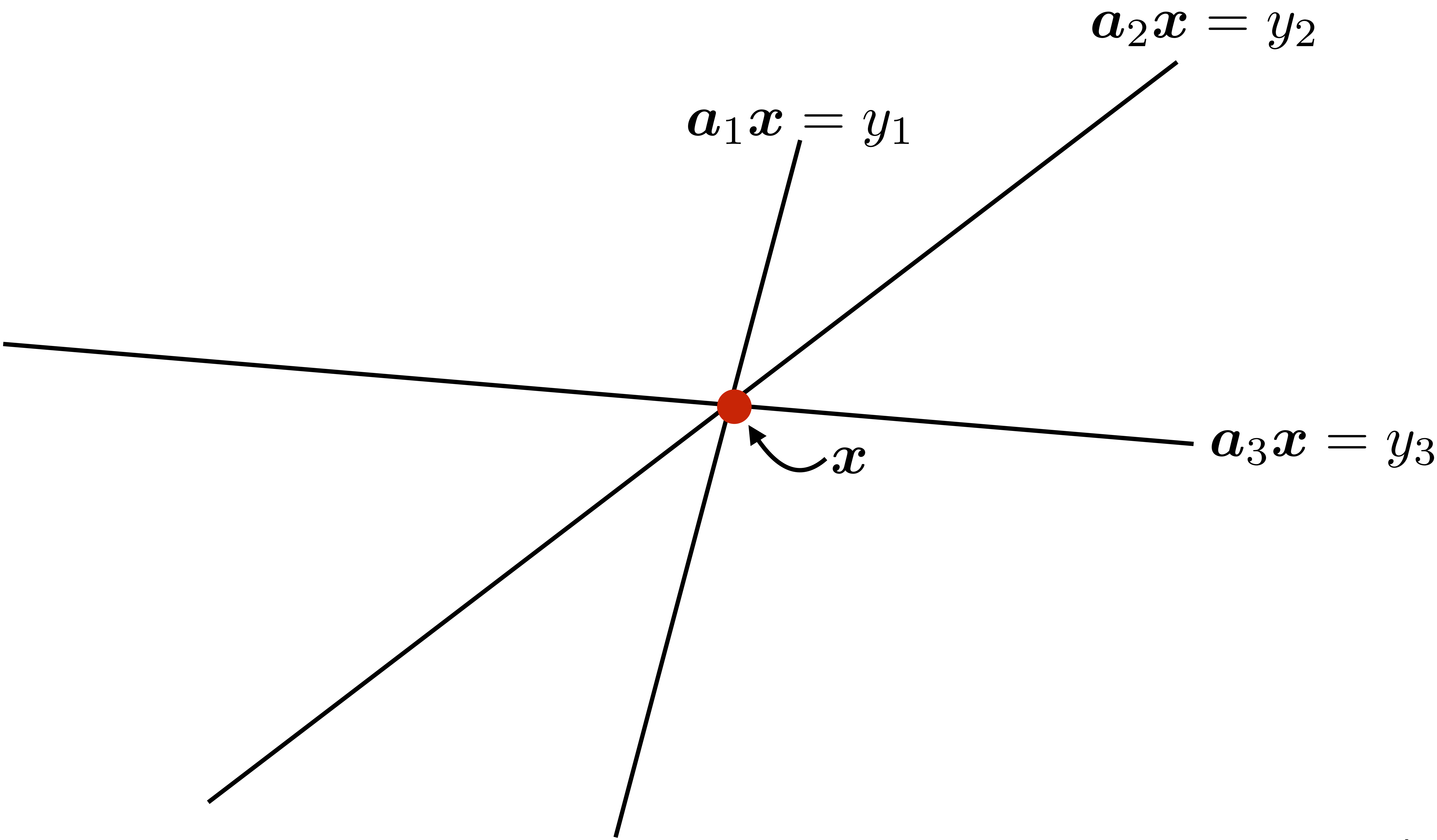
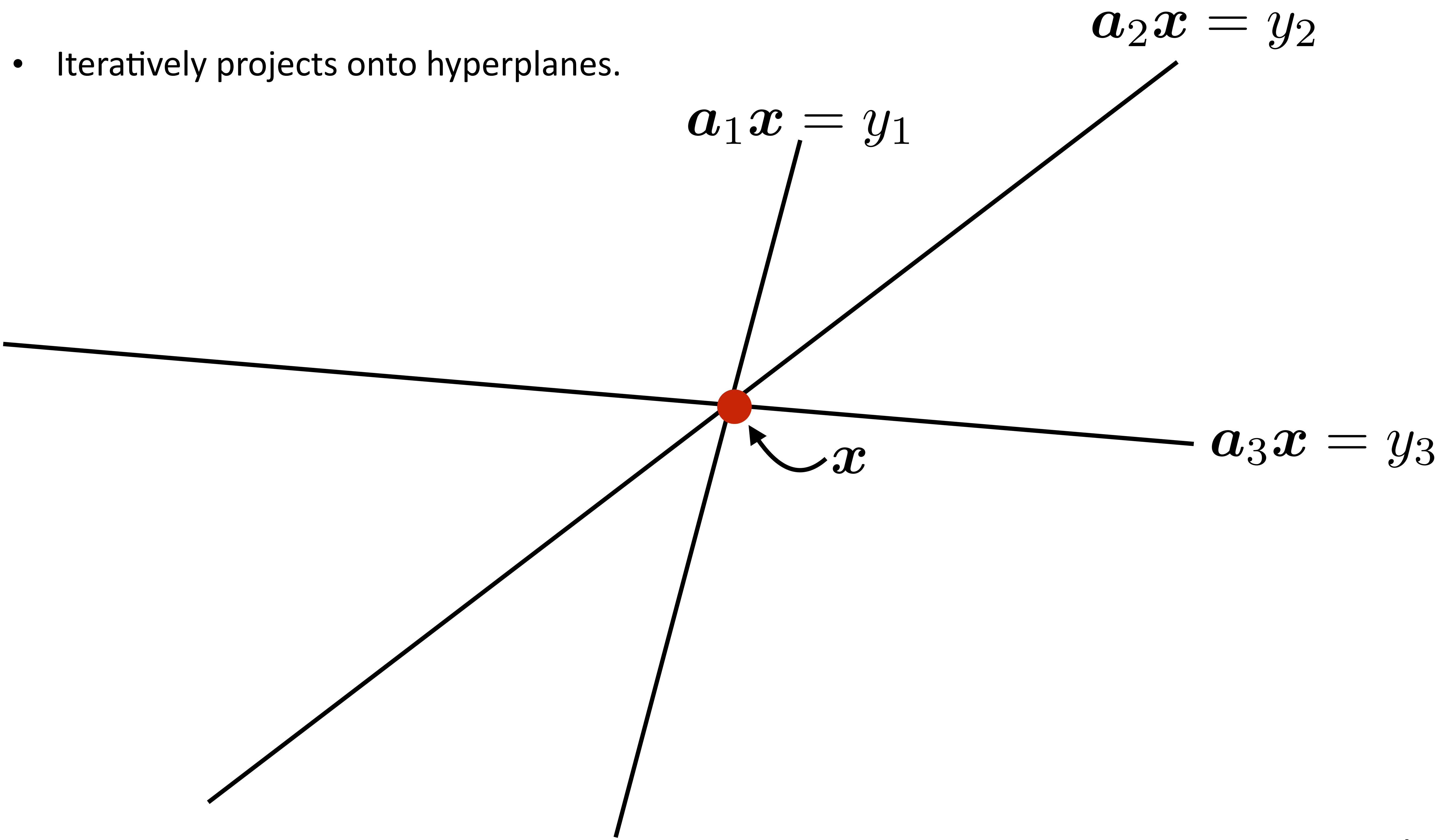


Kaczmarz Algorithm — Iterative Projections

- Noiseless case: $\boldsymbol{y} = \boldsymbol{A}\boldsymbol{x}$ encodes a system of m equations.
- Iteratively projects onto hyperplanes.



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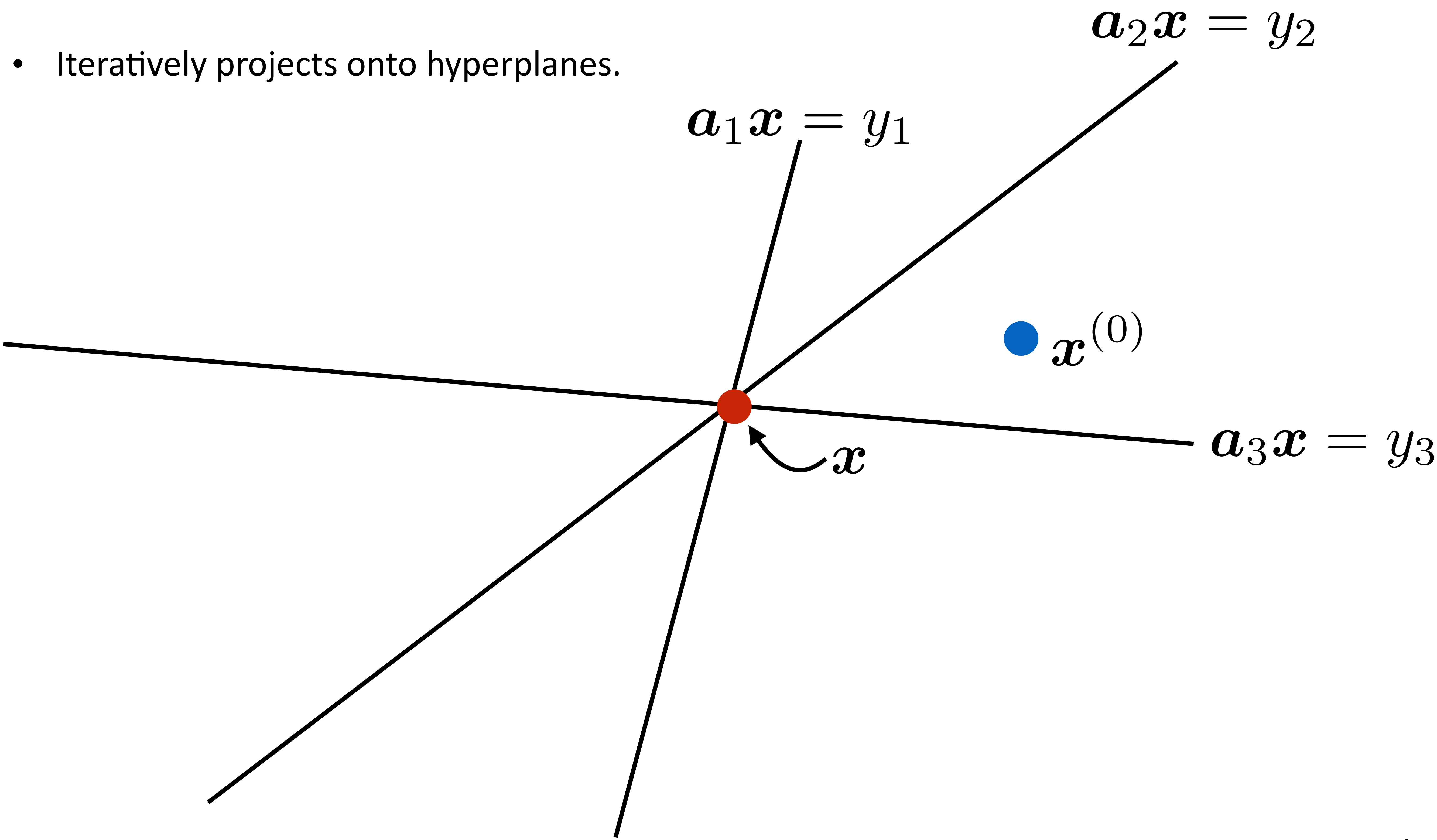

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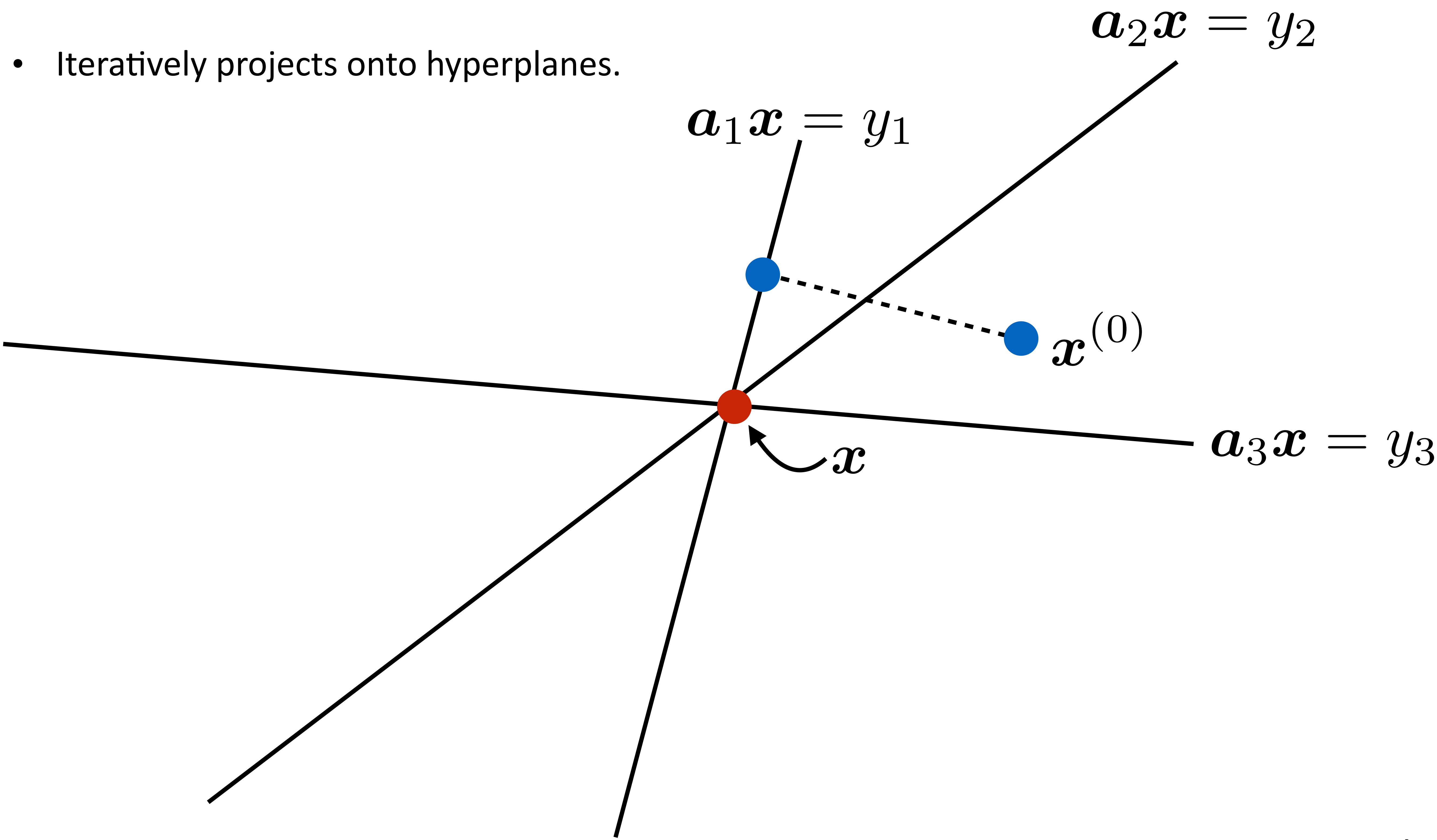

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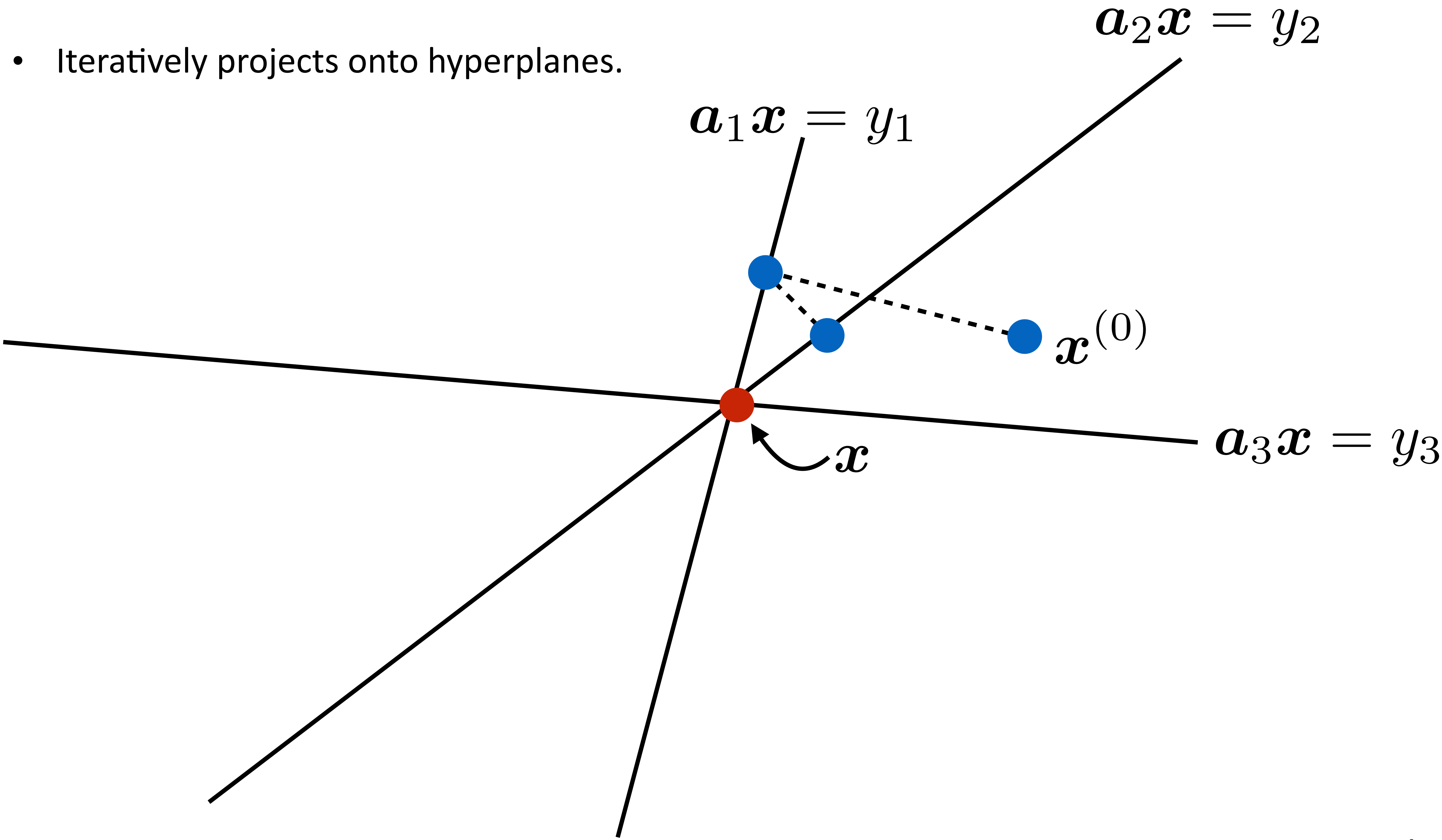

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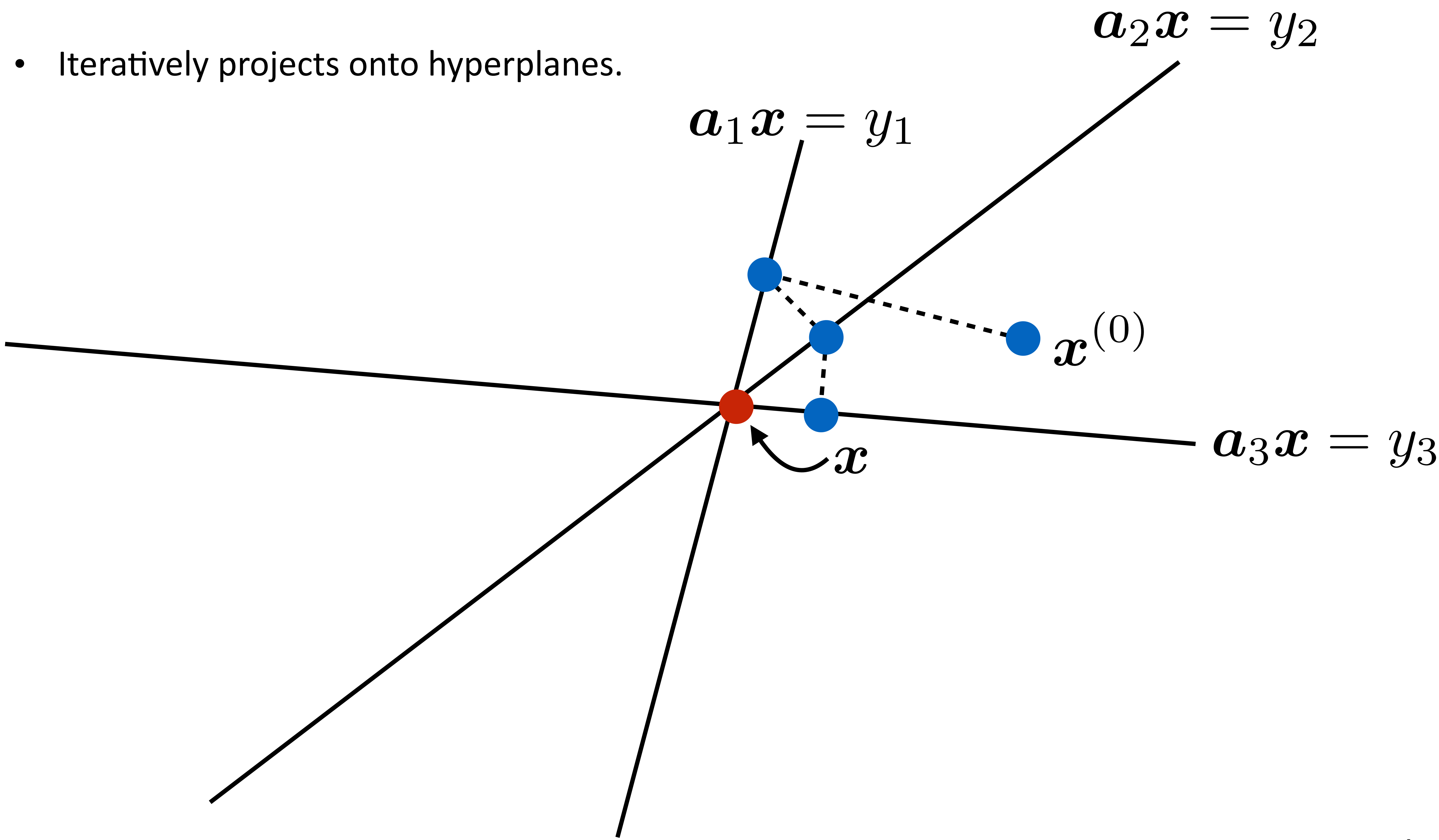

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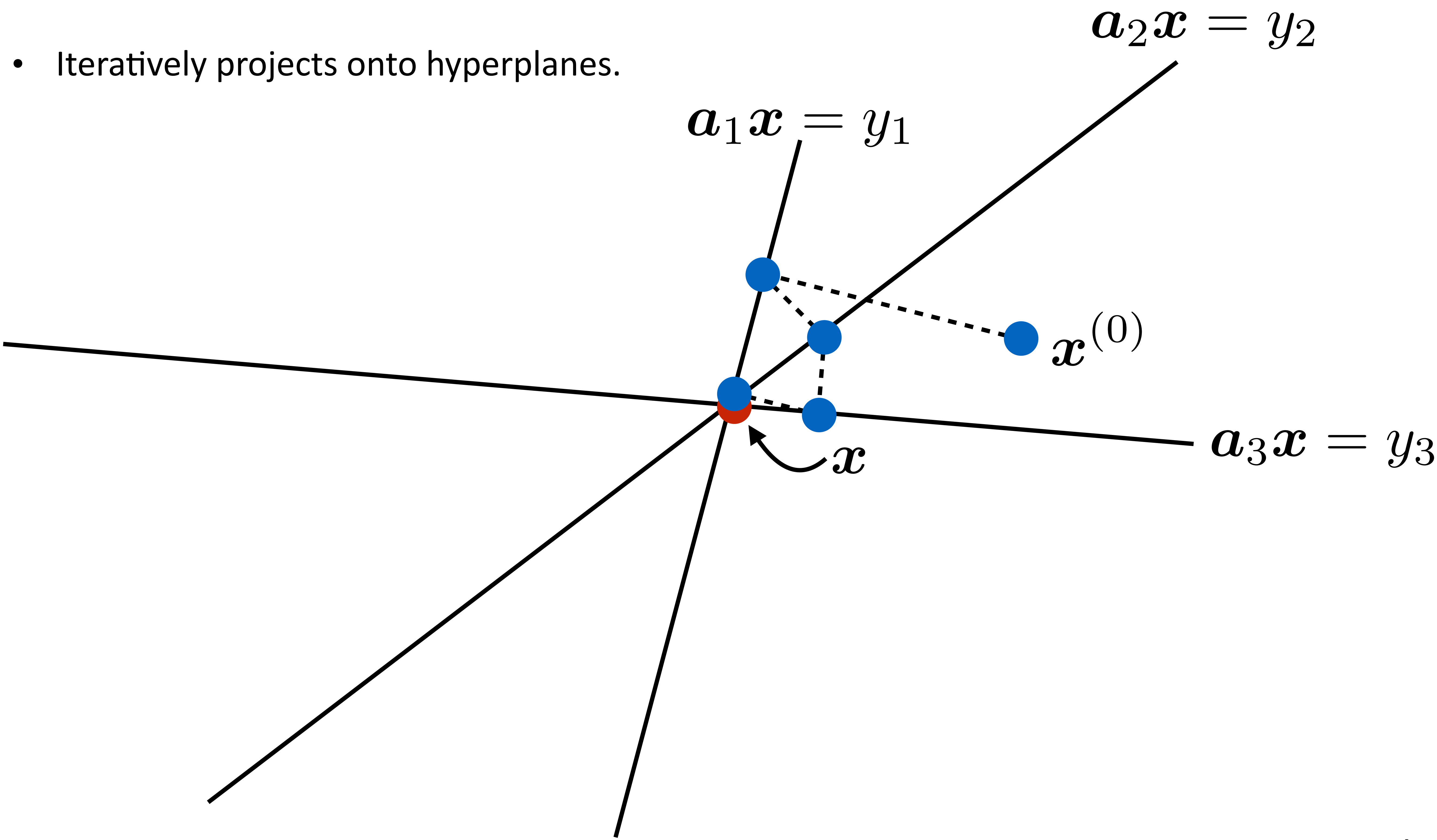

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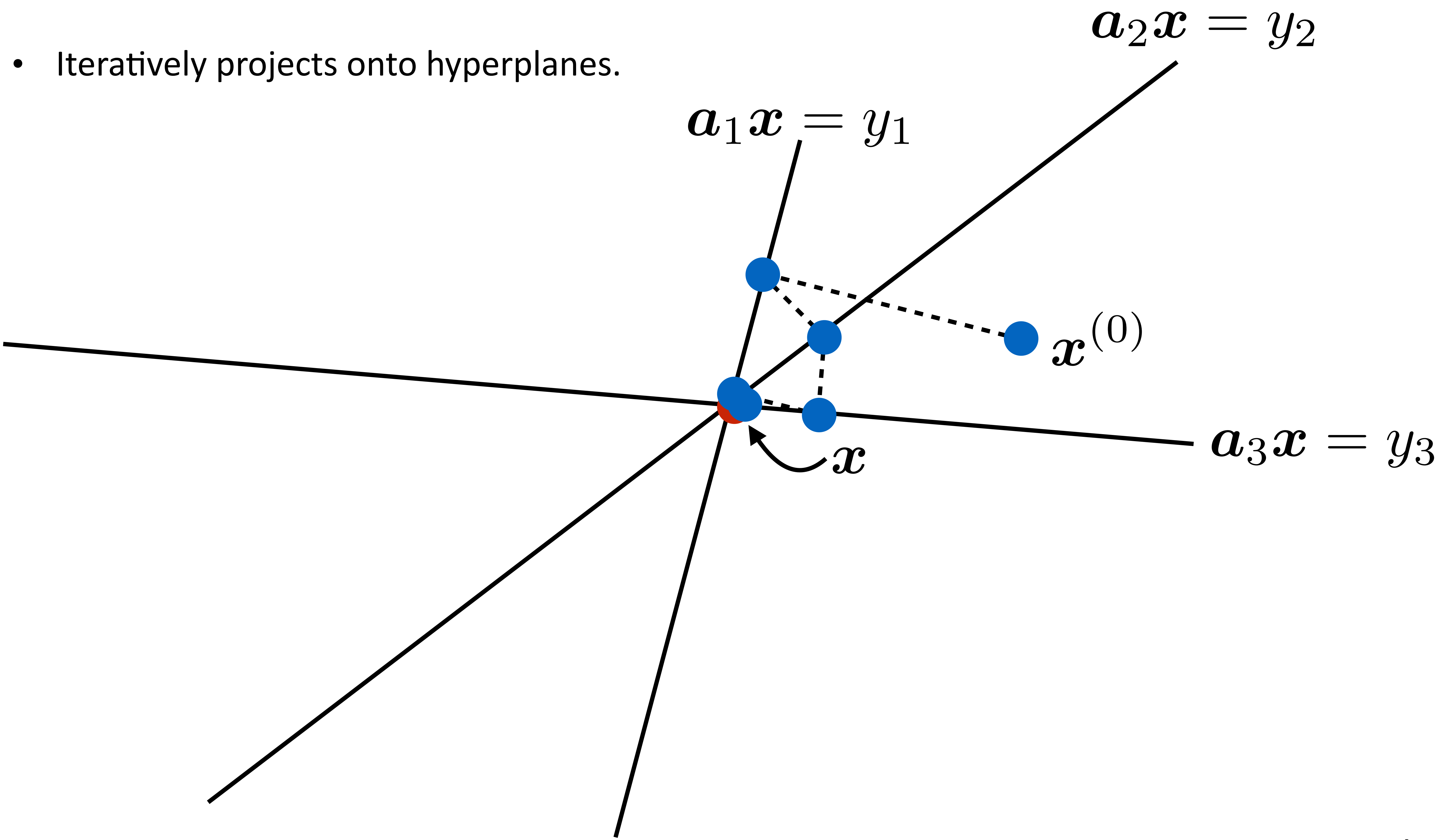

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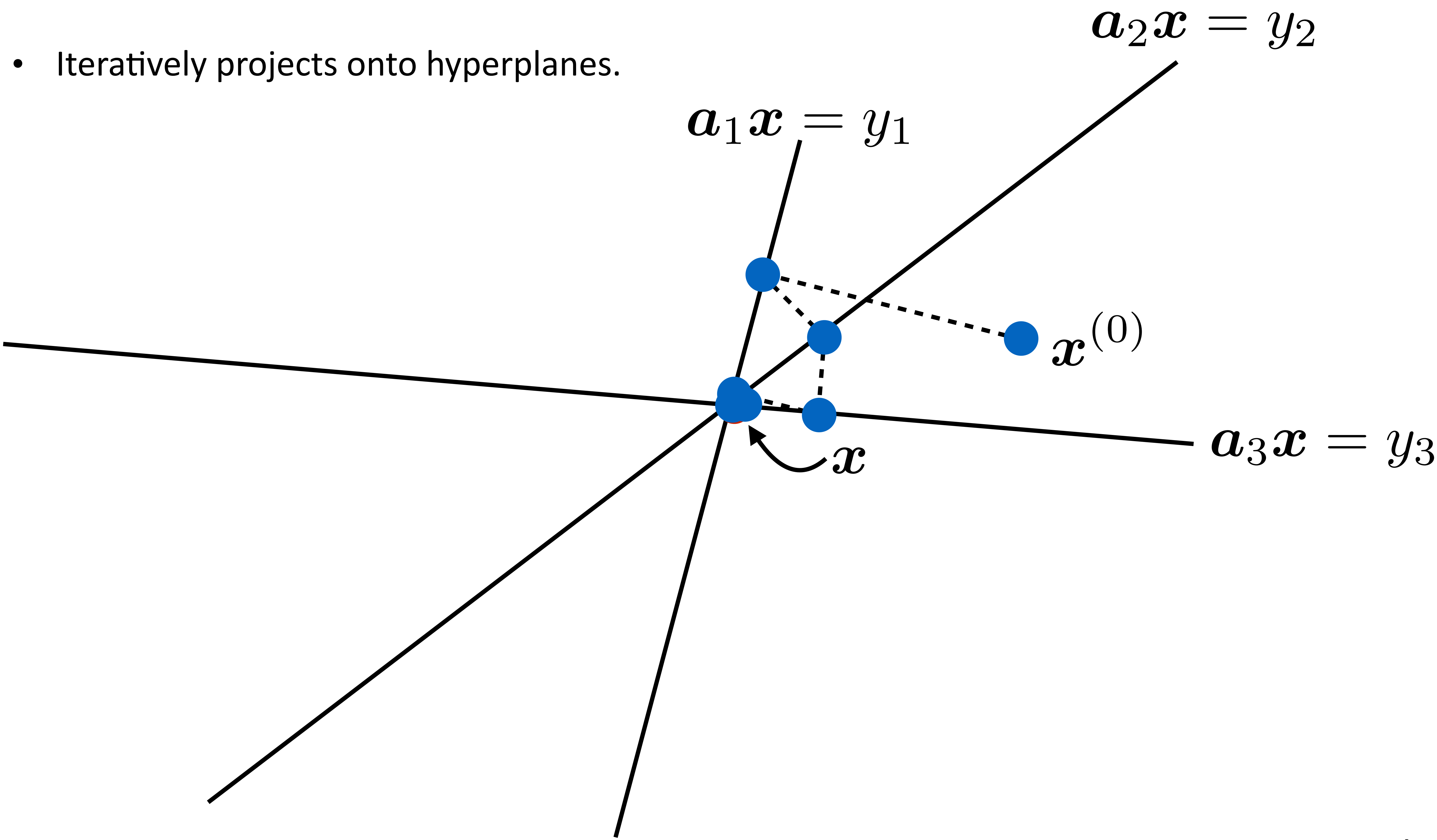


Kaczmarz Algorithm

- Iterative algorithm introduced by S. Kaczmarz (1937)
- Also known as algebraic reconstruction technique (ART)
- Special case of projection onto convex sets (POCS)

Pseudocode

Initialize arbitrary $\boldsymbol{x}^{(0)}$.

For $k = 1$ to N_{iter}:

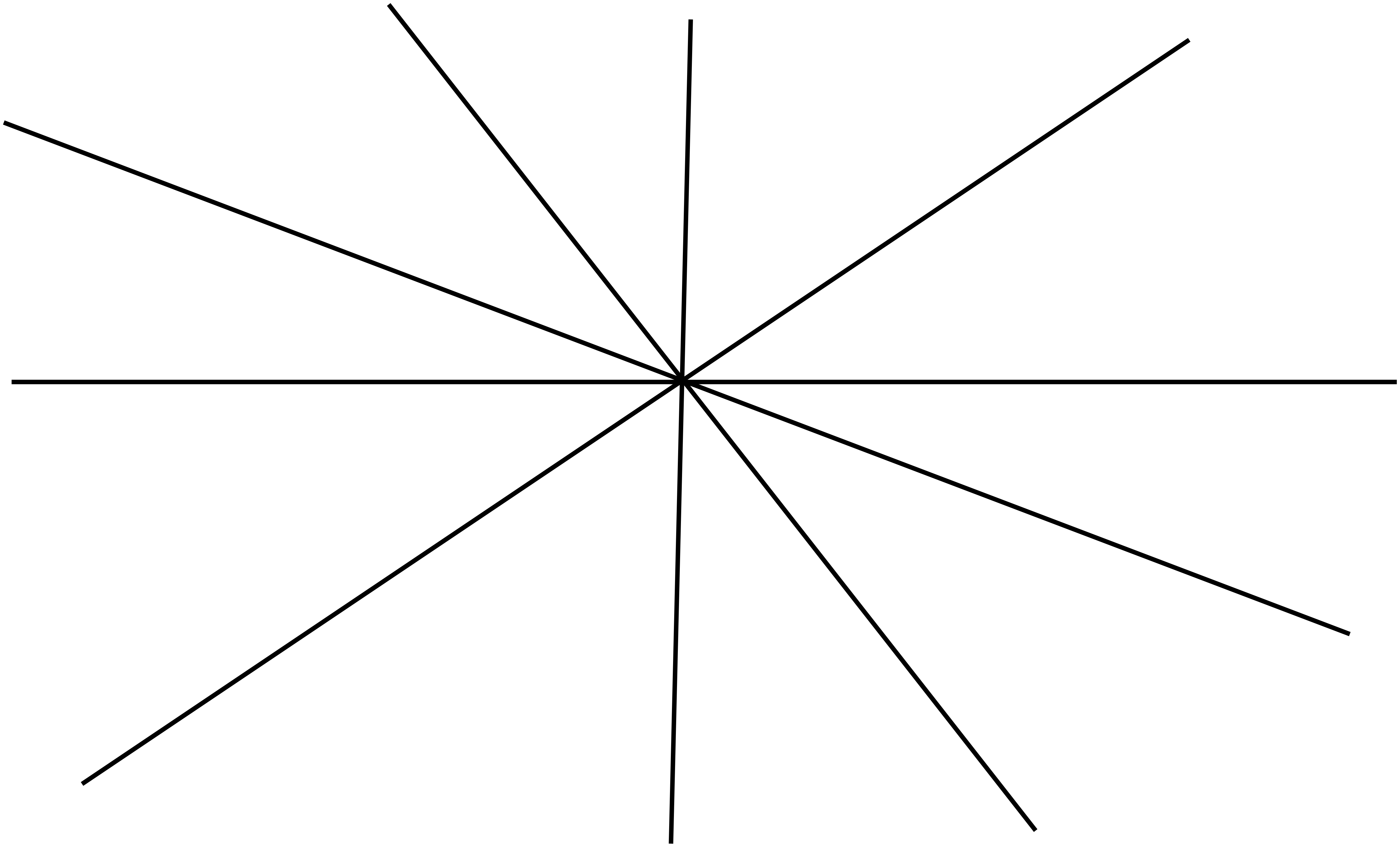
$$r \leftarrow (k \bmod m) + 1$$ *select the next row*

$$\boldsymbol{x}^{(k)} \leftarrow \boldsymbol{x}^{(k-1)} + \frac{y_r - \boldsymbol{a}_r^T \boldsymbol{x}^{(k-1)}}{||\boldsymbol{a}_r||^2} \boldsymbol{a}_r$$ *projection*

$$\widehat{\boldsymbol{x}} \leftarrow \boldsymbol{x}^{(N_{\mathrm{iter}})}$$

- Can be extended to find least squares estimate from noisy measurements (Zouzias & Freris 2013)

Order matters!



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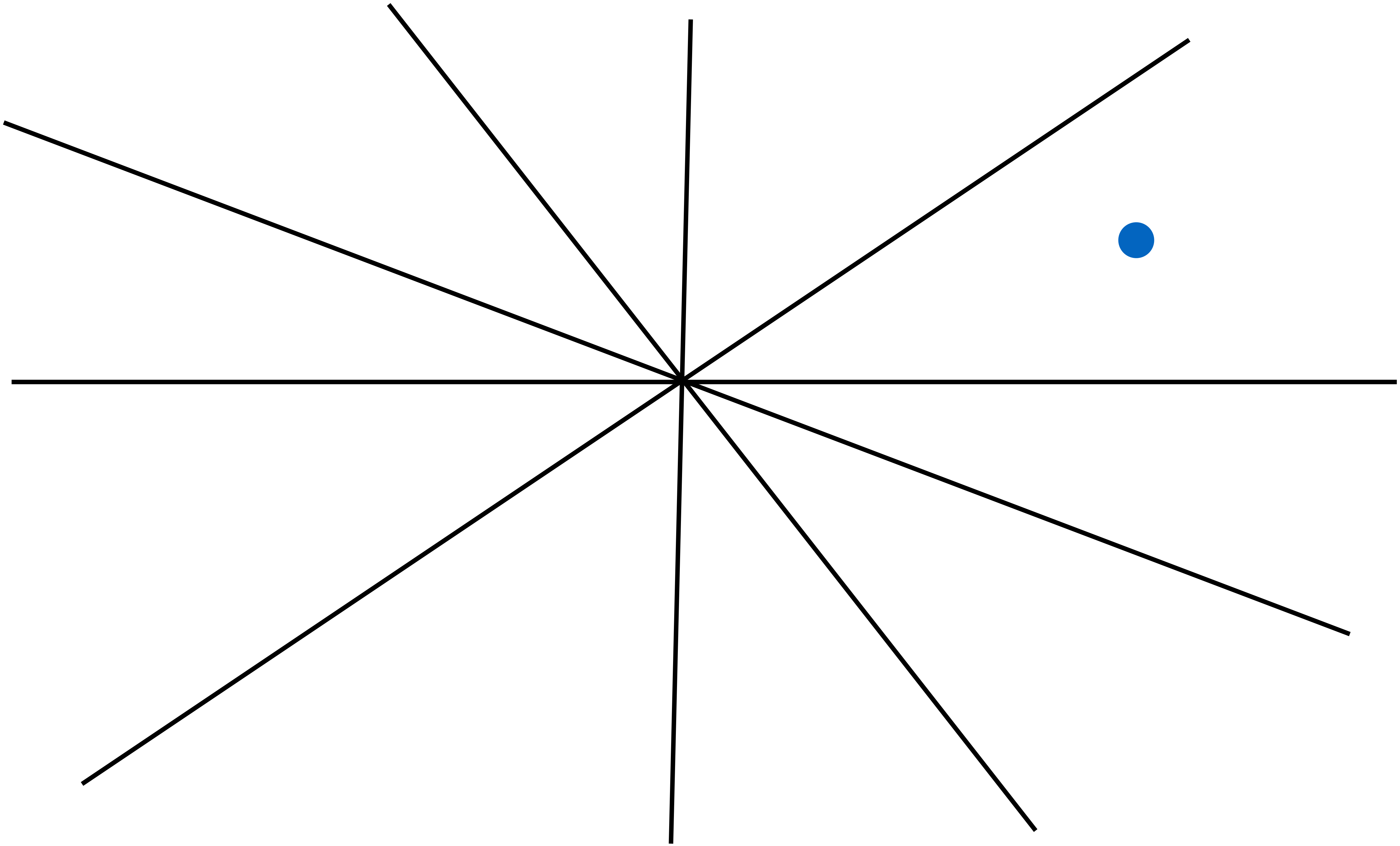

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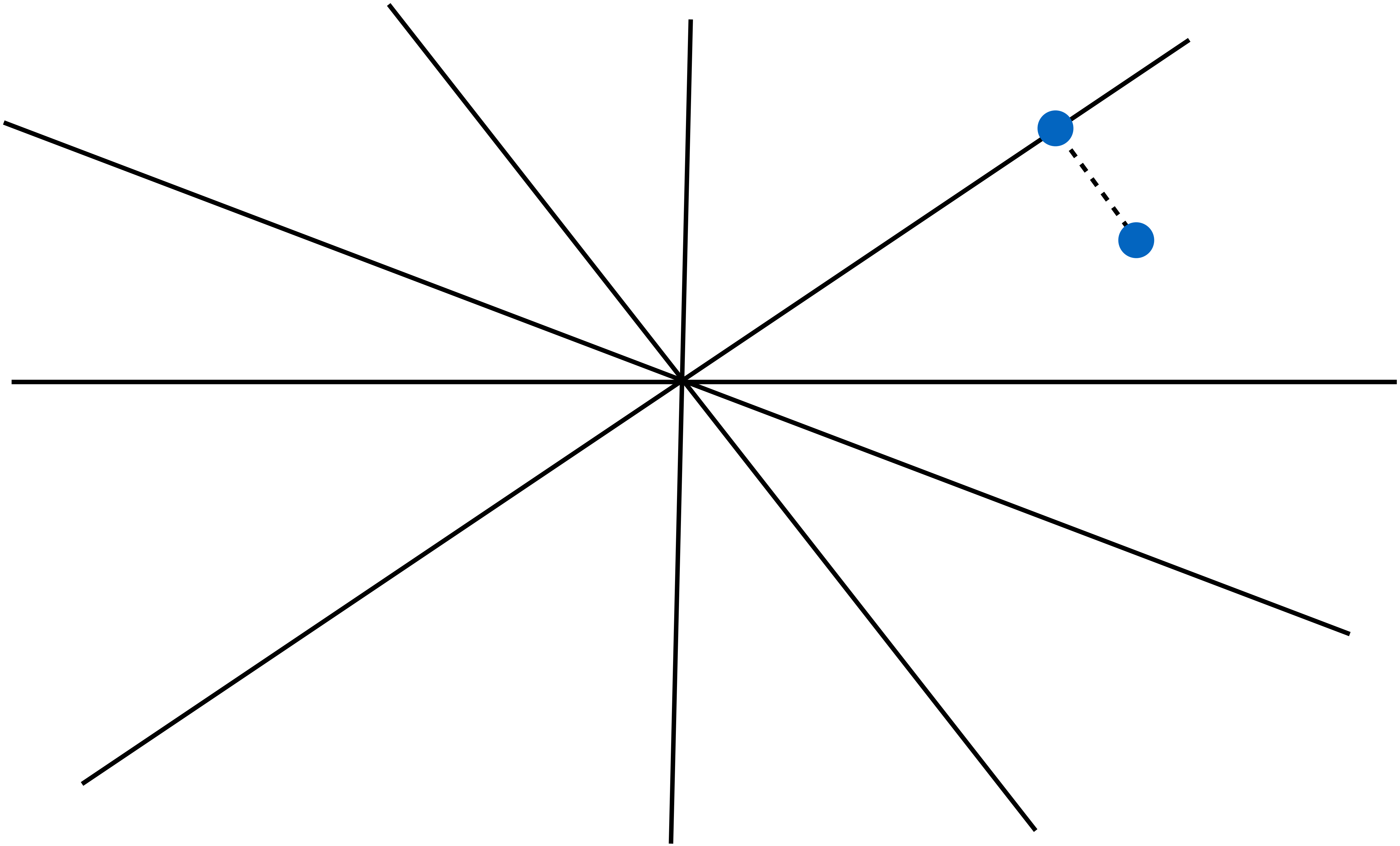

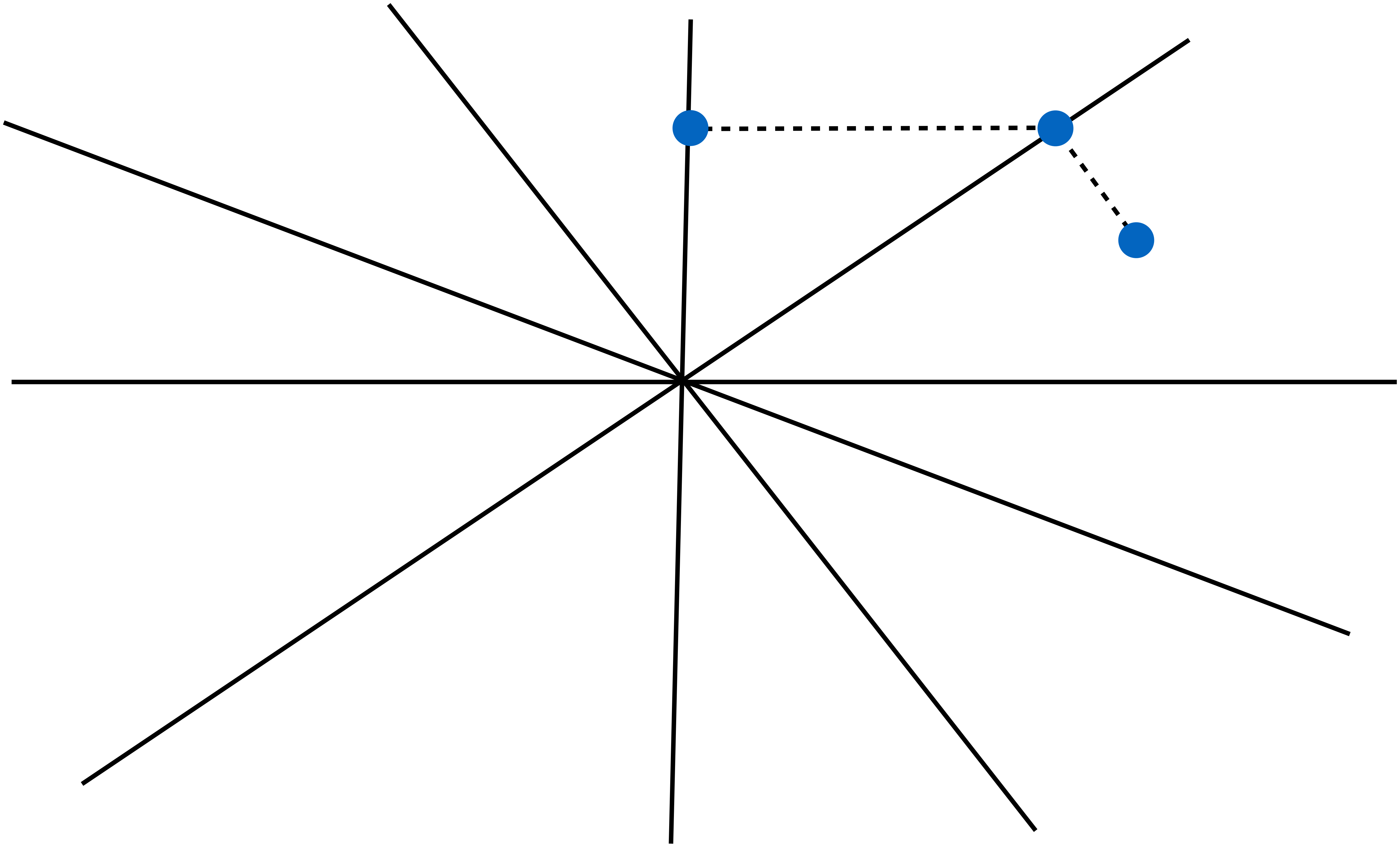

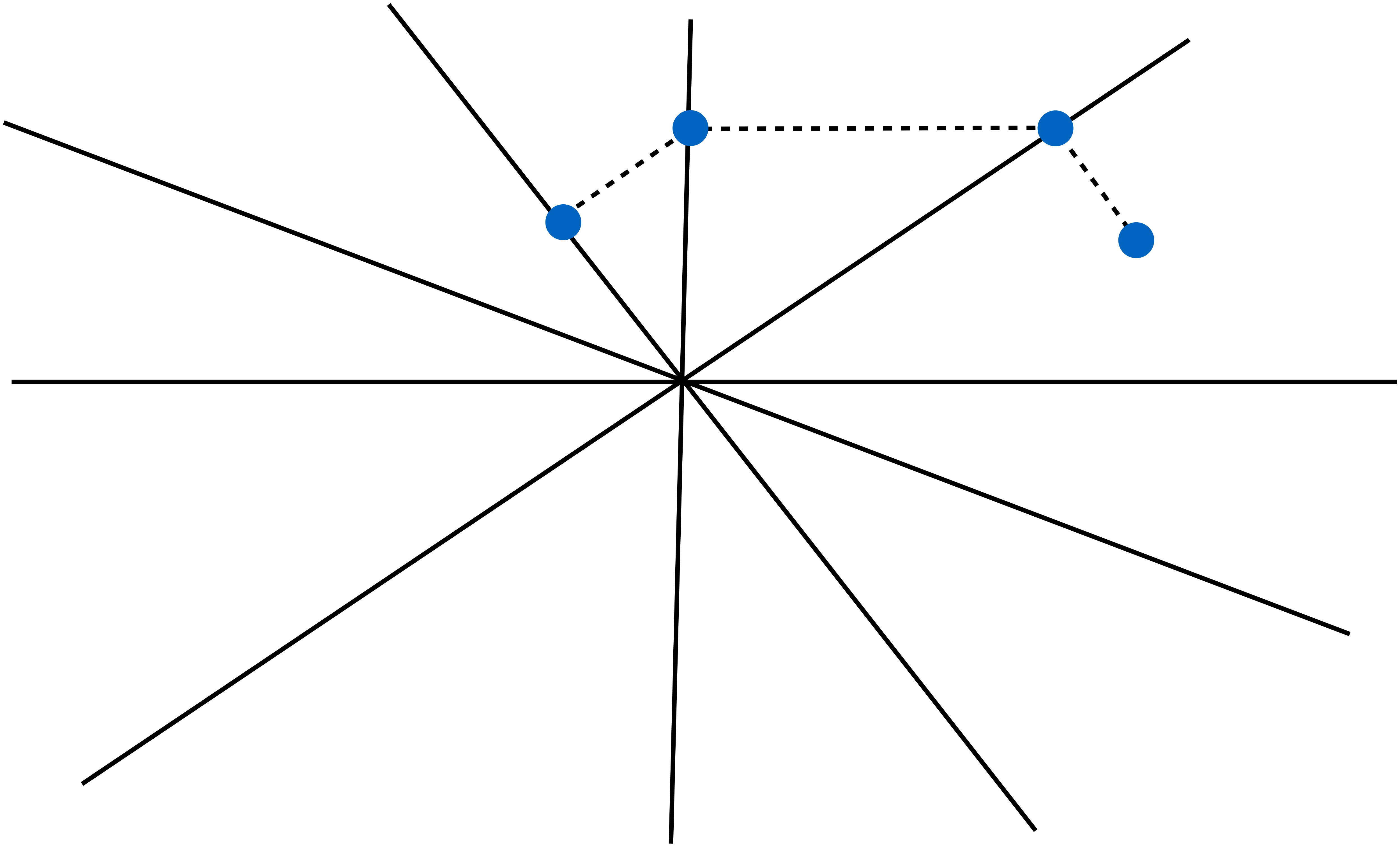

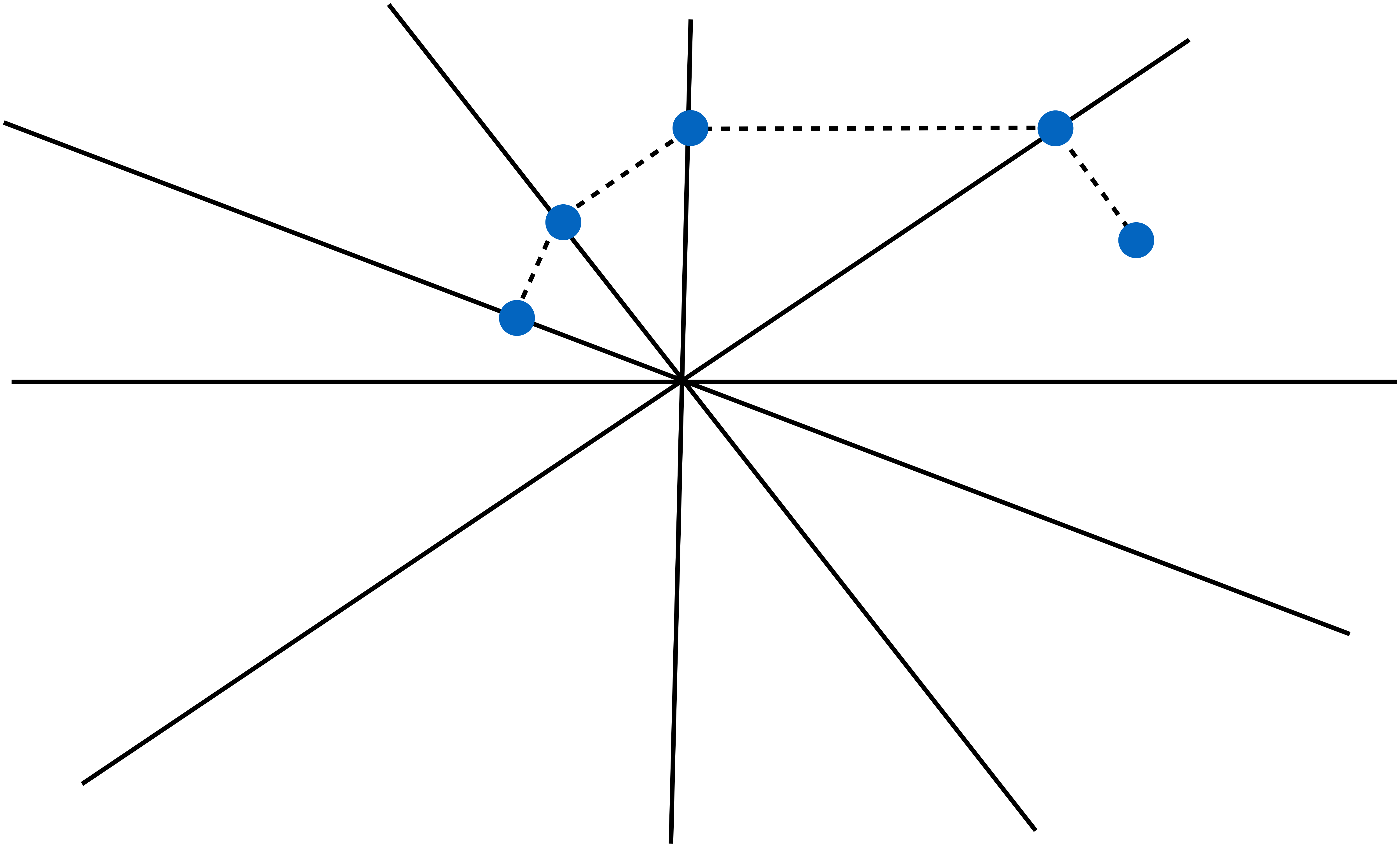

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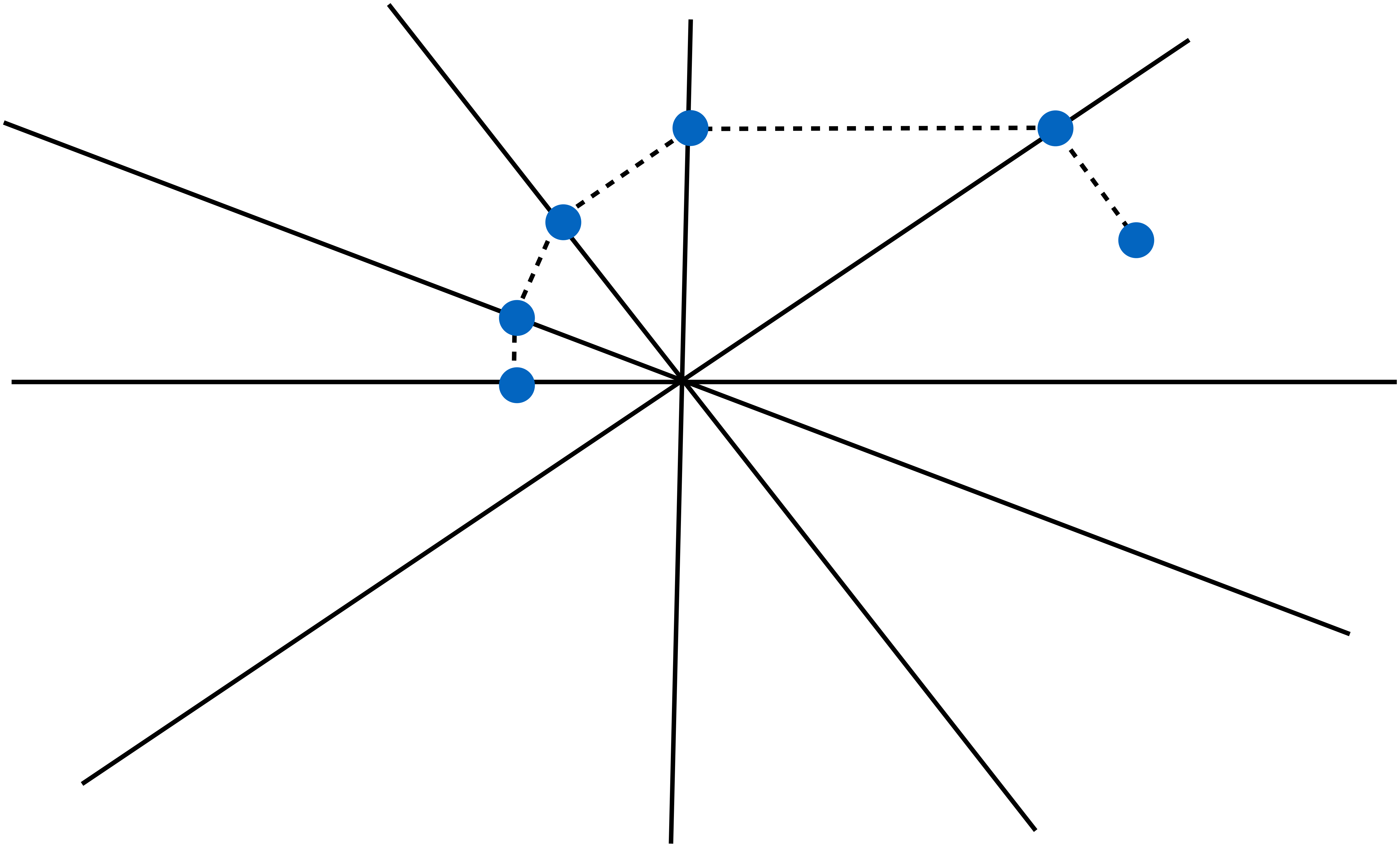

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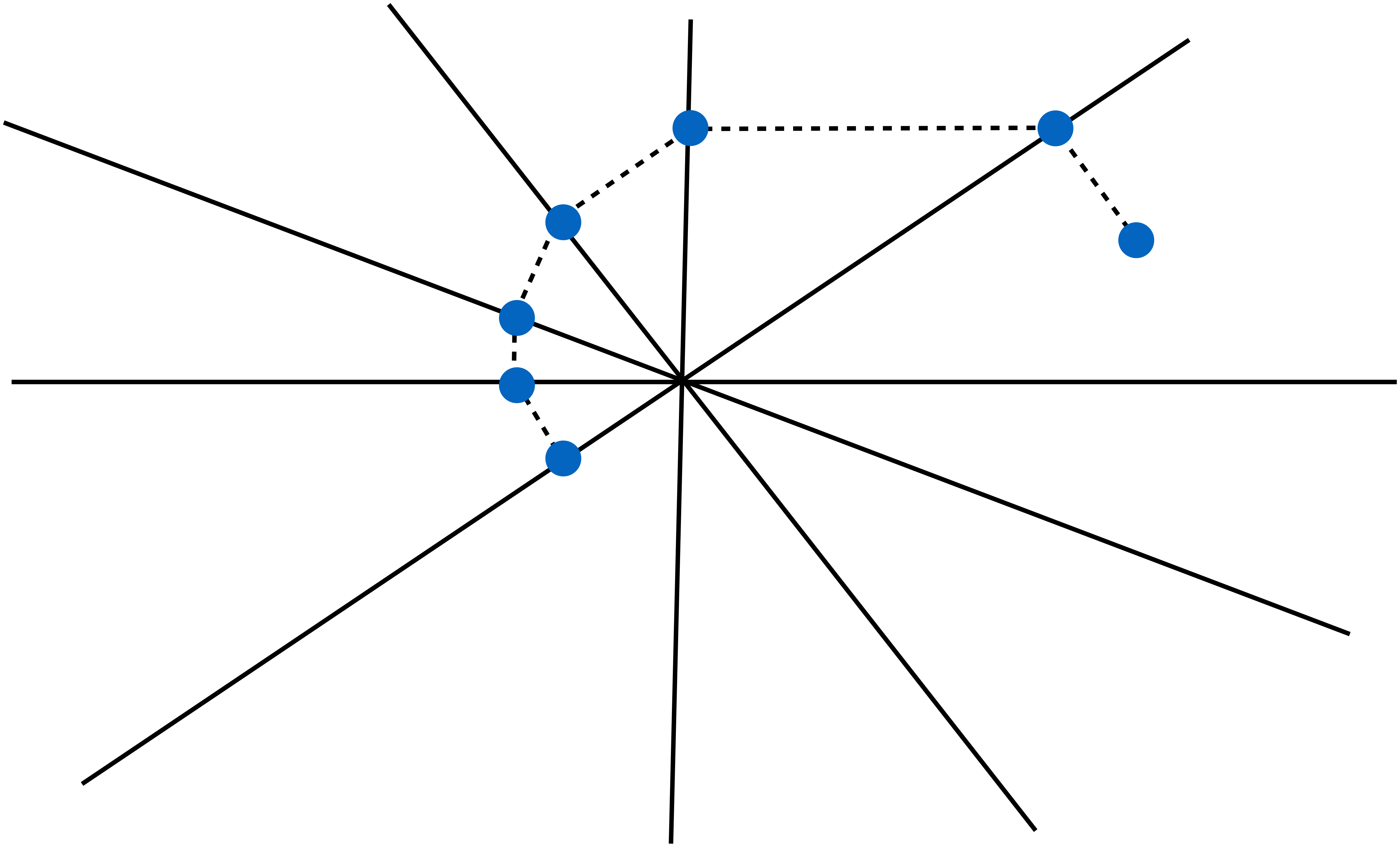

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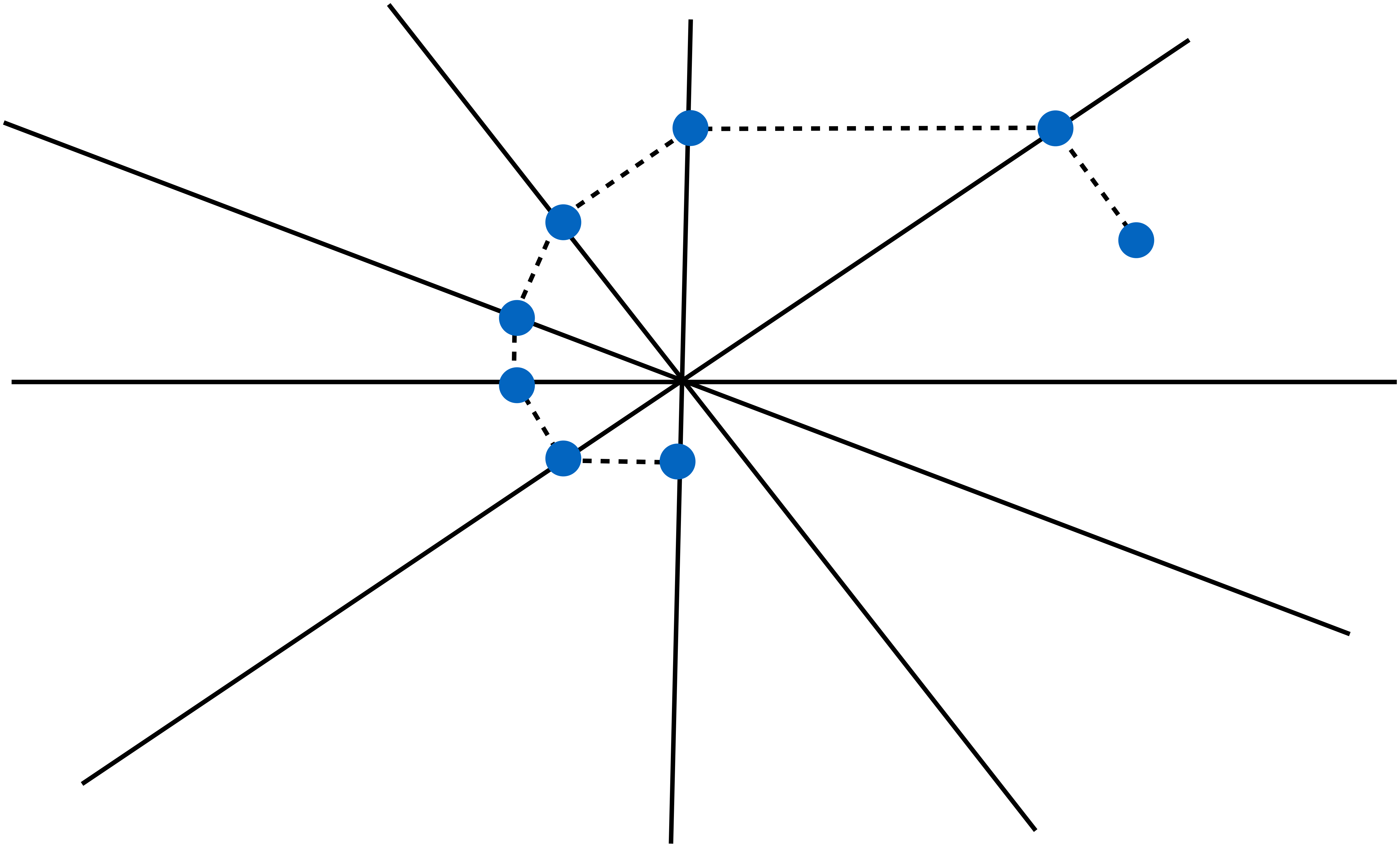

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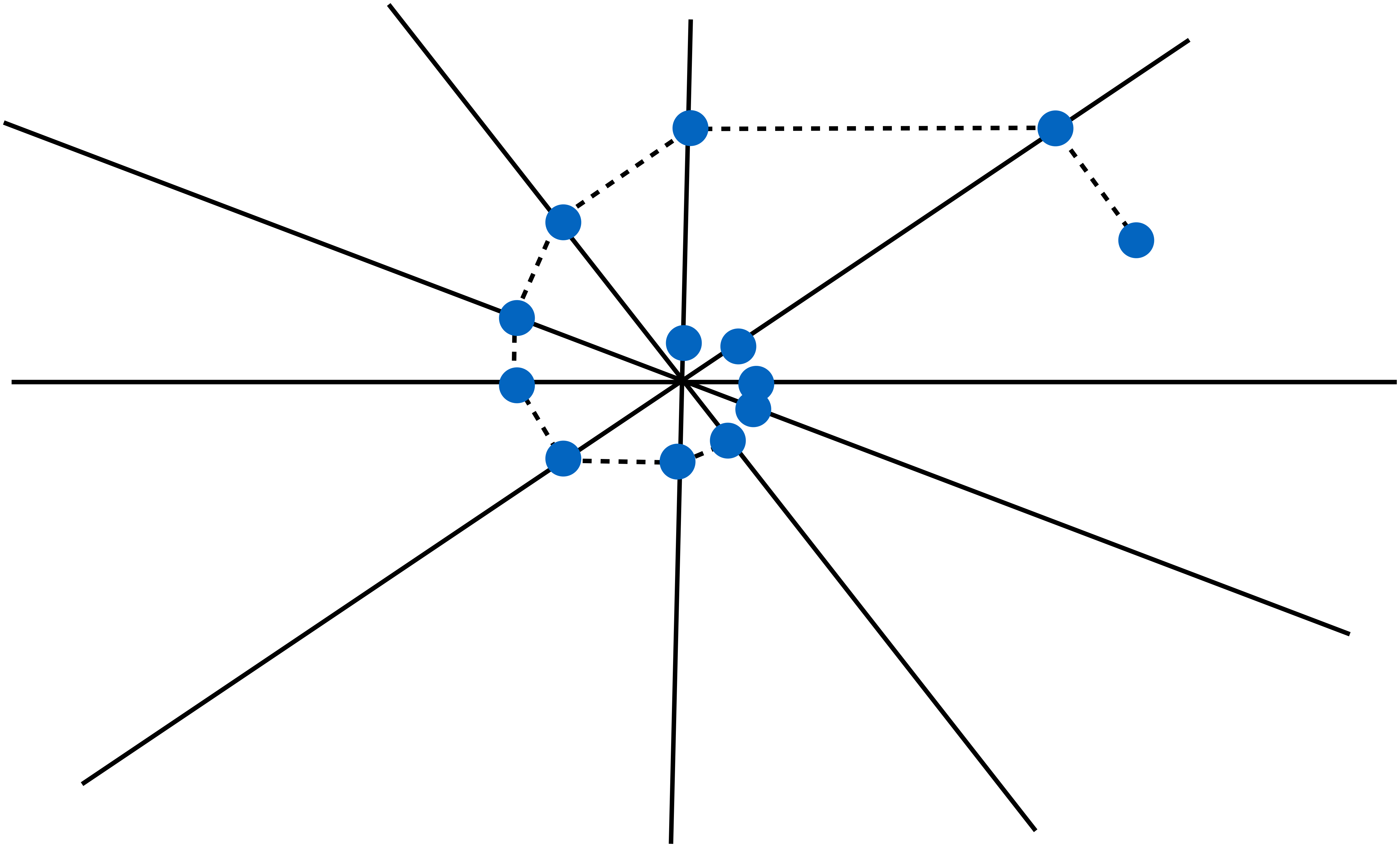

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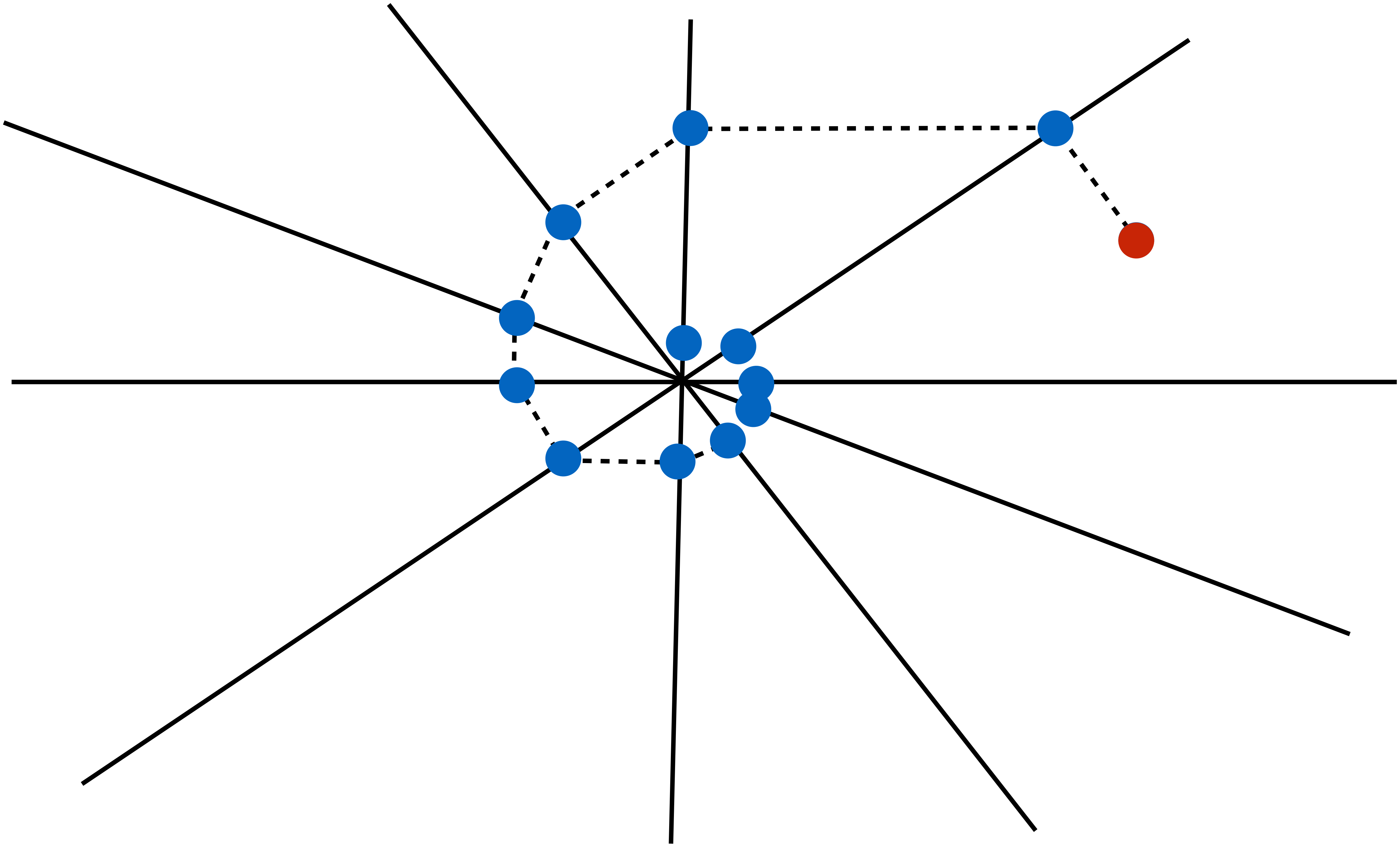

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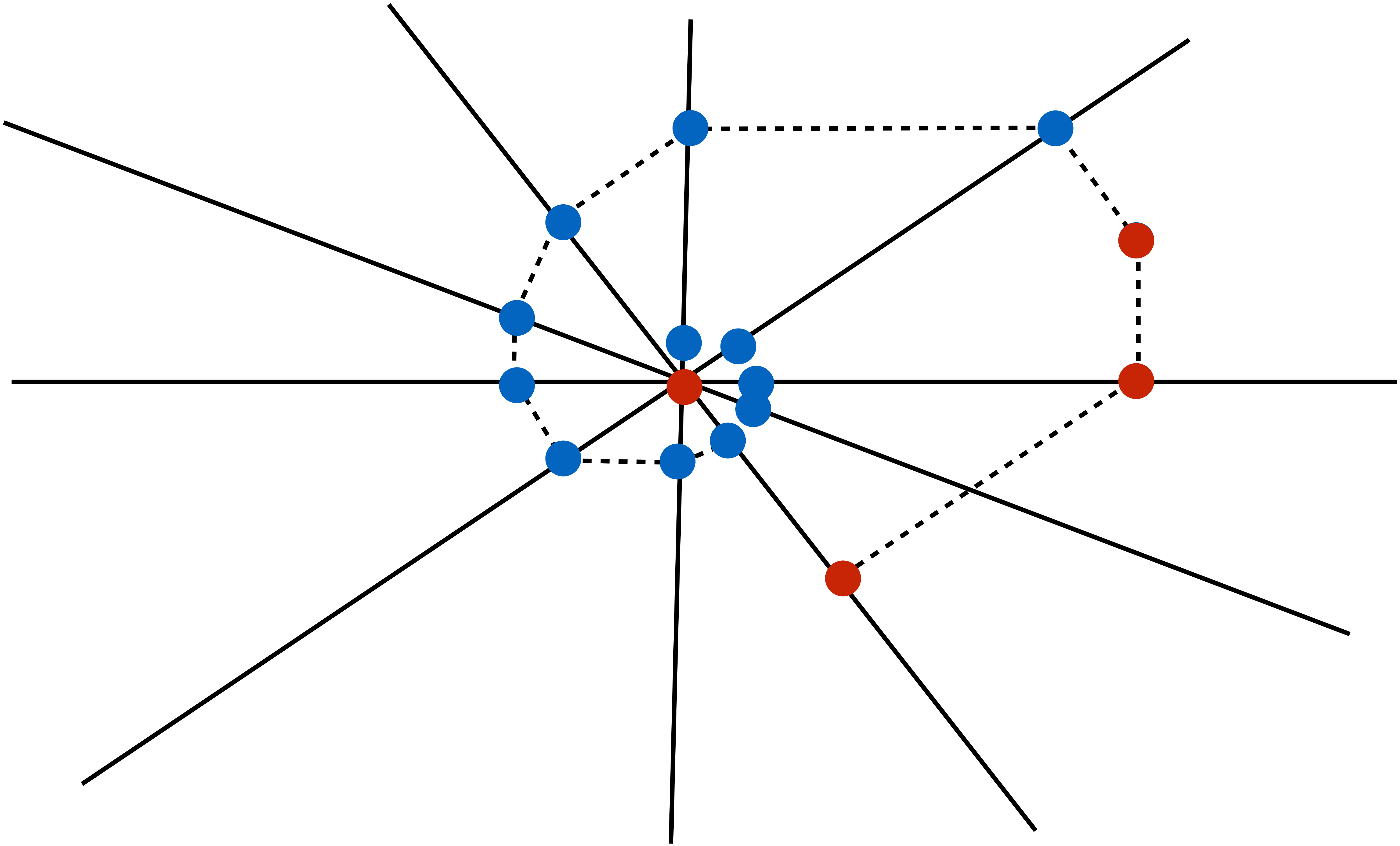


IF YOU USE THE WRONG ROW ORDER
INSTRUCTO
YOU'RE GONNA HAVE A BAD TIME
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Solution: Randomized Kaczmarz

- Strohmer and Vershynin (2009) proposed randomizing the order:

Choose row $\boldsymbol{a}_i$ with probability proportional to $||\boldsymbol{a}_i||^2$.

- Guarantees exponential convergence:

$$\frac{\mathbb{E}||\boldsymbol{x}^{(N)} - \boldsymbol{x}||^2}{||\boldsymbol{x}^{(0)} - \boldsymbol{x}||^2} \leq (1 - \underbrace{\kappa(A)}_{||A||_F ||A^{-1}||_2}{}^{-2})^N$$

- Works for arbitrary probabilities by preconditioning, so we assume row i chosen with probability p_i.

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Related work

- Error bounds for ***inconsistent systems*** (Needell 2012)
- ***Almost-sure*** convergence (Chen & Powell 2012)
- Extension to find ***least-square solution*** in noise (Zouzias & Freris 2013)
- ***Block*** Kaczmarz (Needell & Tropp 2014)

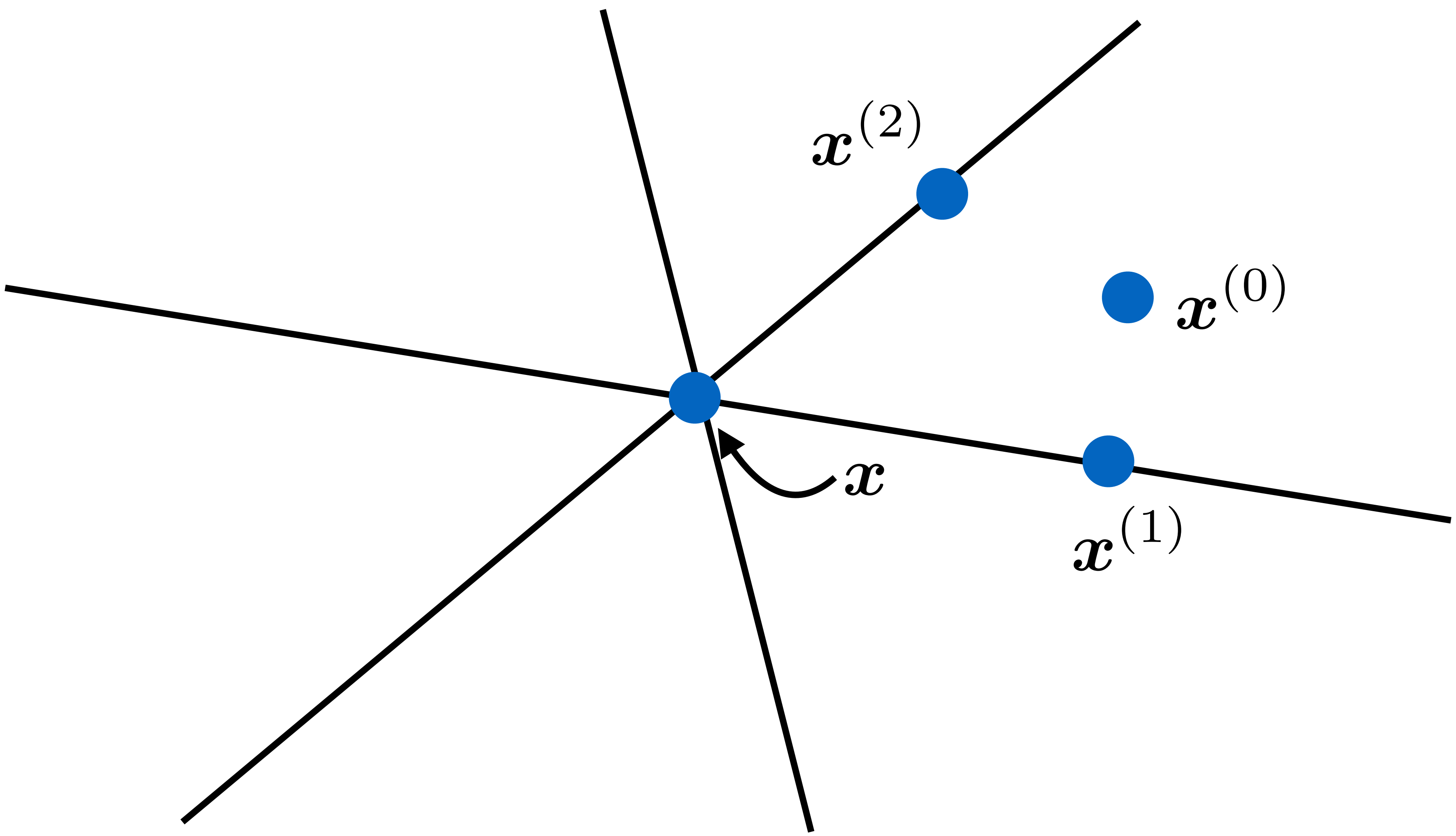
This talk

1. Exact MSE formula and decay rate

2. Optimization of row selection probabilities

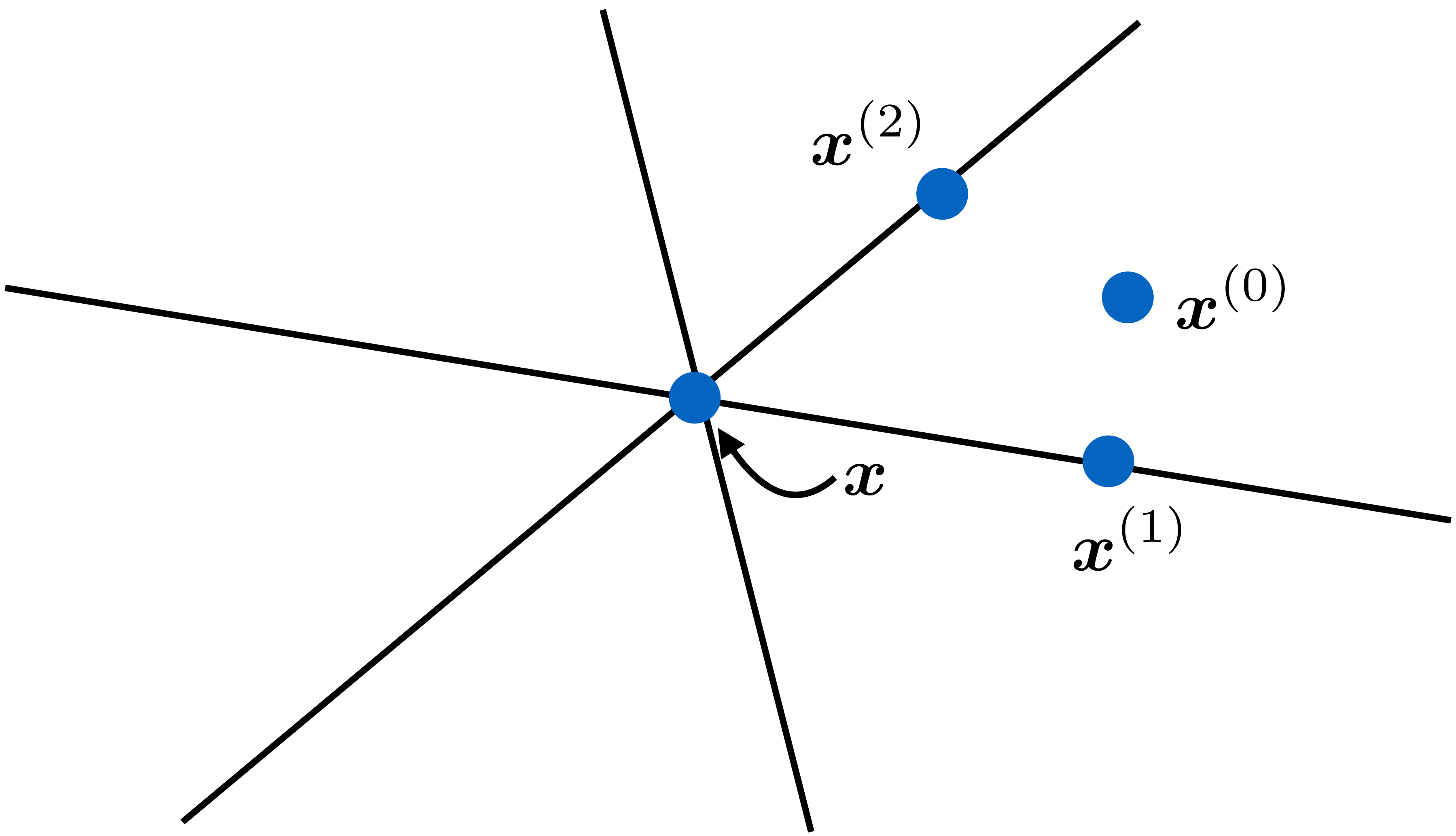
3. “Quenched error exponent”

$$\boldsymbol{x}^{(k)} = \boldsymbol{x}^{(k-1)} + \frac{y_r - \boldsymbol{a}_r^T \boldsymbol{x}^{(k-1)}}{||\boldsymbol{a}_r||^2} \boldsymbol{a}_r$$



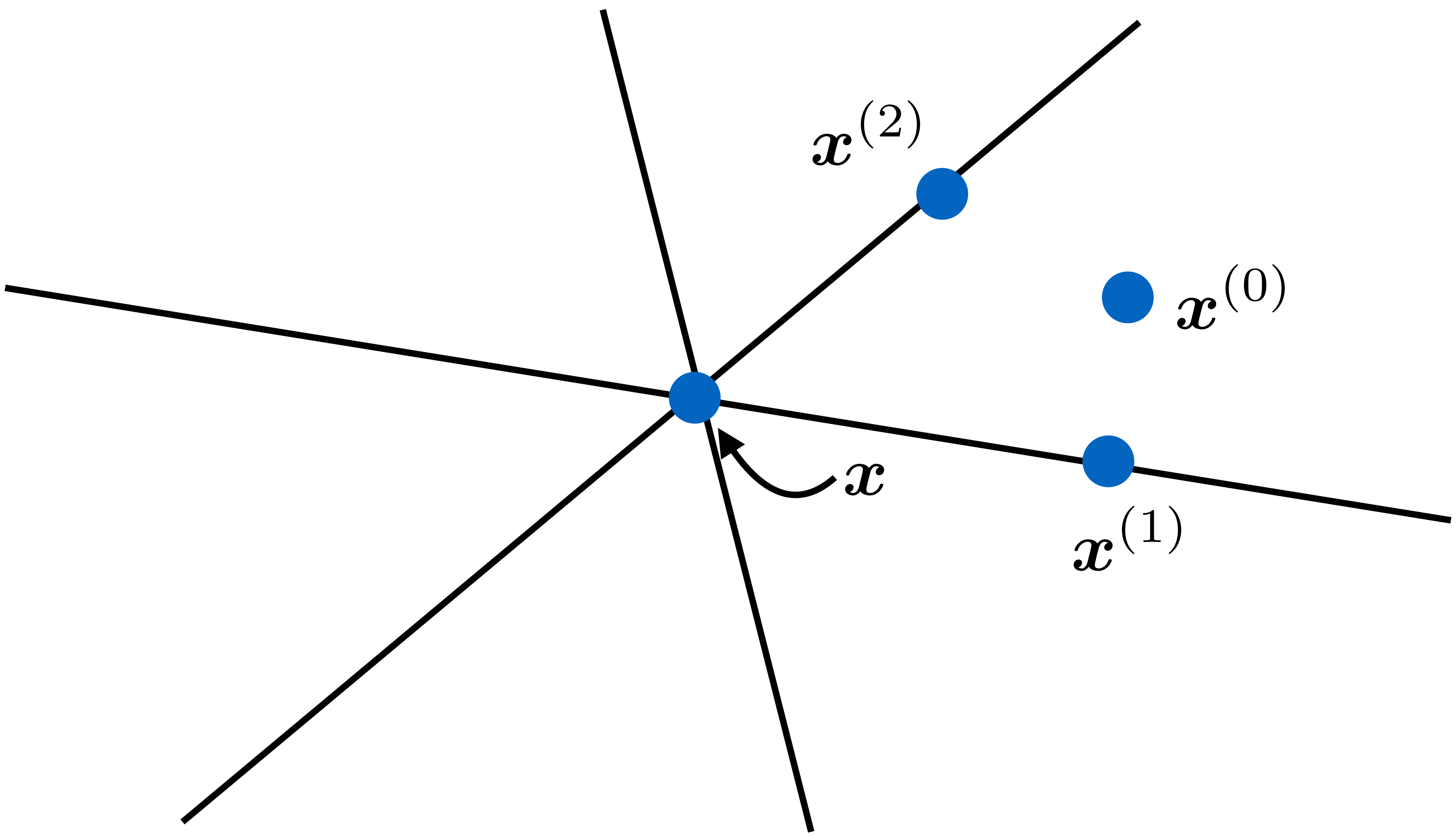
Exact MSE Formula

$$\boldsymbol{x}^{(k)} - \boldsymbol{x} = \boldsymbol{x}^{(k-1)} - \boldsymbol{x} + \frac{y_r - \boldsymbol{a}_r^T \boldsymbol{x}^{(k-1)}}{||\boldsymbol{a}_r||^2}\boldsymbol{a}_r$$



Exact MSE Formula

$$(\boldsymbol{x}^{(k)} - \boldsymbol{x}) = (\boldsymbol{x}^{(k-1)} - \boldsymbol{x}) - \frac{\boldsymbol{a}_r^T(\boldsymbol{x}^{(k-1)} - \boldsymbol{x})}{||\boldsymbol{a}_r||^2}\boldsymbol{a}_r$$



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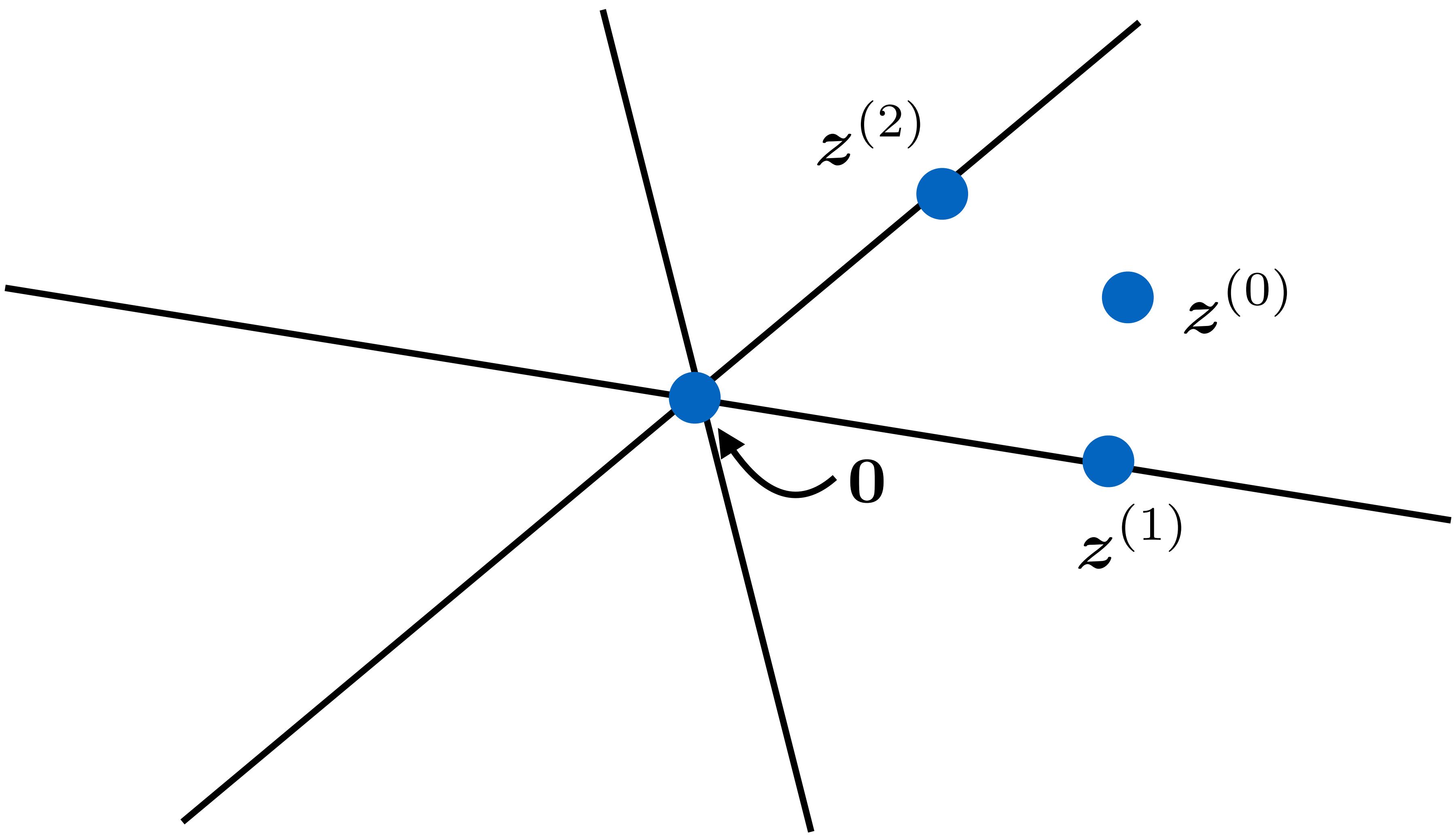
$\boldsymbol{z}^{(k)} = Q_k \boldsymbol{z}^{(k-1)}$ where $\boldsymbol{Q}_k = \left(I - \frac{\boldsymbol{a}_r \boldsymbol{a}_r^T}{||\boldsymbol{a}_r||^2}\right)$



Exact MSE Formula

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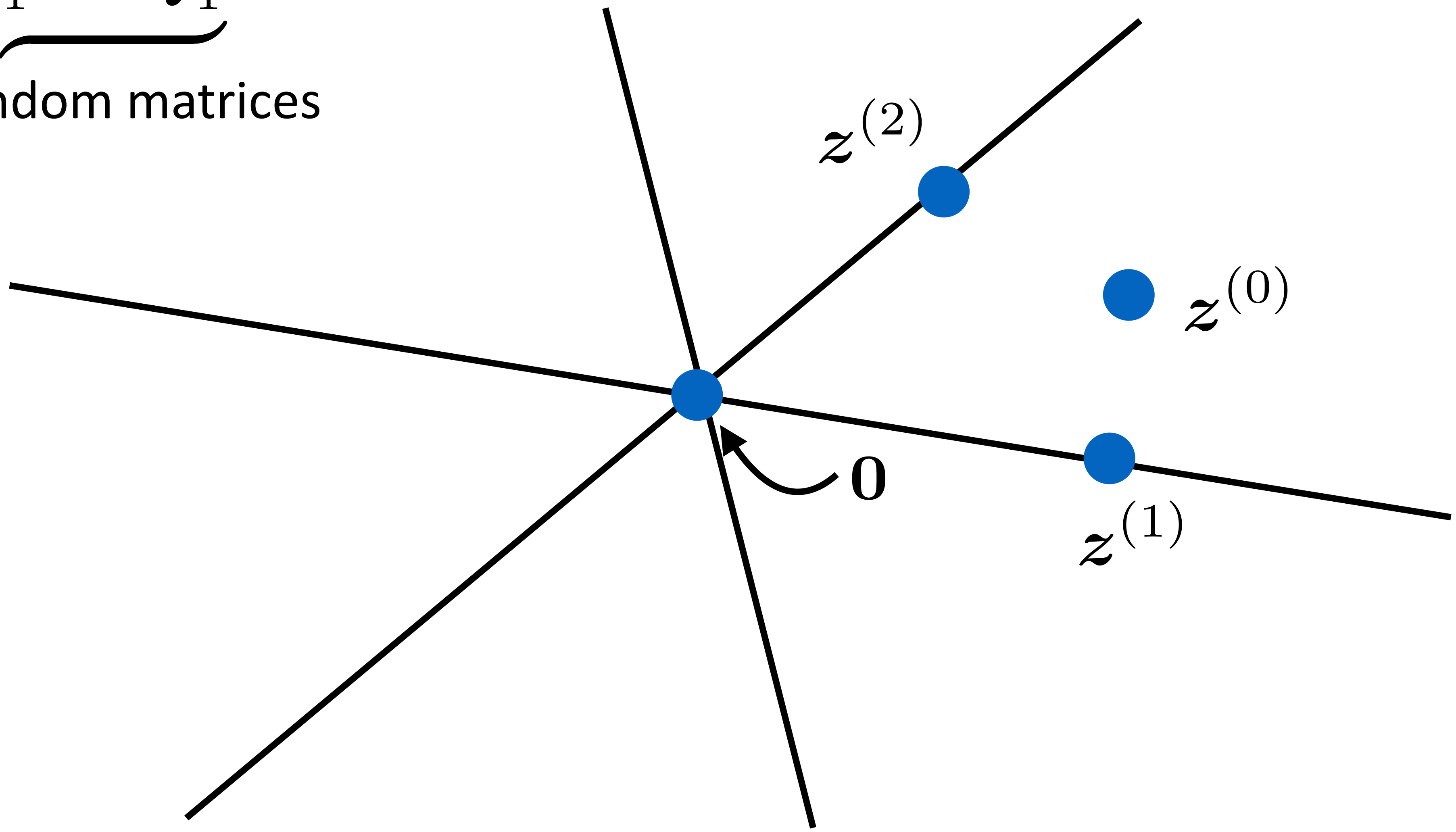
$$\boldsymbol{z}^{(k)} = \underbrace{\boldsymbol{Q}_k \boldsymbol{Q}_{k-1} \cdots \boldsymbol{Q}_1}_{\text{product of random matrices}} \boldsymbol{z}^{(0)}$$



Exact MSE Formula

Proposition (A.-Wang-Lu 2014)

$$\mathrm{MSE}_N = \mathrm{vec}\, \boldsymbol{I}^T (\mathbb{E}\boldsymbol{Q} \otimes \boldsymbol{Q})^N \,\mathrm{vec}(\boldsymbol{z}^{(0)} \boldsymbol{z}^{(0)T})$$

where $\mathbb{E}\boldsymbol{Q} \otimes \boldsymbol{Q} = \sum_i p_i \left(\boldsymbol{I} - \frac{\boldsymbol{a}_i \boldsymbol{a}_i^T}{||\boldsymbol{a}_i||^2} \right)^{\otimes 2}$

vec — vectorization operator; stack columns of matrix into vector.

$\otimes$ — matrix Kronecker product.

Proof sketch

$$\underbrace{\mathbb{E}||\boldsymbol{z}^{(N)}||^2}_{\text{MSE}} = \mathbb{E}||\boldsymbol{Q}_N \boldsymbol{Q}_{N-1} \cdots \boldsymbol{Q}_1 \boldsymbol{z}^{(0)}||^2$$

$$= \mathbb{E}\boldsymbol{z}^{(0)T} \boldsymbol{Q}_1 \boldsymbol{Q}_2 \cdots \boldsymbol{Q}_N \boldsymbol{Q}_N \cdots \boldsymbol{Q}_2 \boldsymbol{Q}_1 \boldsymbol{z}^{(0)}$$

$$= \mathbb{E}\,\mathrm{trace}(\boldsymbol{Q}_1 \boldsymbol{Q}_2 \cdots \boldsymbol{Q}_N \boldsymbol{Q}_N \cdots \boldsymbol{Q}_2 \boldsymbol{Q}_1 \boldsymbol{z}^{(0)} \boldsymbol{z}^{(0)T})$$

$$= \mathbb{E}\,\mathrm{vec}(\boldsymbol{Q}_1 \boldsymbol{Q}_2 \cdots \boldsymbol{Q}_N \boldsymbol{Q}_N \cdots \boldsymbol{Q}_2 \boldsymbol{Q}_1)^T \,\mathrm{vec}(\boldsymbol{z}^{(0)} \boldsymbol{z}^{(0)T})$$

Proof sketch

Matrix identities

$$\mathrm{vec}(ABC) = (C^T \otimes A)\,\mathrm{vec}(B)$$

$$\mathrm{trace}(AB) = \mathrm{vec}(A)^T\,\mathrm{vec}(B)$$

$$\mathrm{trace}\,AB = \mathrm{trace}\,BA$$

$$= \mathbb{E}\,\mathrm{vec}(\boldsymbol{Q}_1\boldsymbol{Q}_2\cdots\boldsymbol{Q}_N\boldsymbol{Q}_N\cdots\boldsymbol{Q}_2\boldsymbol{Q}_1)^T\,\mathrm{vec}(\boldsymbol{z}^{(0)}\boldsymbol{z}^{(0)T})$$

Exact MSE formula

$$
\begin{aligned}
&\mathrm{MSE}_N \\
&= \mathbb{E}\{\mathrm{vec}(\boldsymbol{Q}_1\boldsymbol{Q}_2\cdots\boldsymbol{Q}_N\boldsymbol{Q}_N\cdots\boldsymbol{Q}_2\boldsymbol{Q}_1)\}^T\,\mathrm{vec}(\boldsymbol{z}^{(0)}\boldsymbol{z}^{(0)T}) \\
&= \mathbb{E}\{(\boldsymbol{Q}_1\otimes\boldsymbol{Q}_1)\,\mathrm{vec}(\boldsymbol{Q}_2\cdots\boldsymbol{Q}_N\boldsymbol{Q}_N\cdots\boldsymbol{Q}_2)\}^T\,\mathrm{vec}(\boldsymbol{z}^{(0)}\boldsymbol{z}^{(0)T})
\end{aligned}
$$

$\blacksquare$

Exact MSE formula

$$
\begin{aligned}
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&= \{(\mathbb{E}\boldsymbol{Q}\otimes\boldsymbol{Q})^N\,\mathrm{vec}(\boldsymbol{I})\}^T\,\mathrm{vec}(\boldsymbol{z}^{(0)}\boldsymbol{z}^{(0)T})
\end{aligned}
$$

$\blacksquare$

Exact MSE formula

$$
\begin{aligned}
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&= \{(\mathbb{E}\boldsymbol{Q}\otimes\boldsymbol{Q})^N\,\mathrm{vec}(\boldsymbol{I})\}^T\,\mathrm{vec}(\boldsymbol{z}^{(0)}\boldsymbol{z}^{(0)T}) \\
&= \mathrm{vec}\,\boldsymbol{I}^T(\mathbb{E}\boldsymbol{Q}\otimes\boldsymbol{Q})^N\,\mathrm{vec}(\boldsymbol{z}^{(0)}\boldsymbol{z}^{(0)T})\ \blacksquare
\end{aligned}
$$

MSE decays exponentially: $\mathbb{E}||\boldsymbol{z}^{(N)}||^2 = \exp(-\gamma_a N + o(N))$

Error exponent

$$\gamma_a \stackrel{\text{def}}{=} \lim_{N\to\infty} -\frac{1}{N} \log \mathbb{E}||\boldsymbol{z}^{(N)}||^2$$

We can compute the error exponent:

$$\gamma_a = -\log \lambda_{\max} \left(\sum_i p_i \left(\boldsymbol{I} - \frac{\boldsymbol{a}_i \boldsymbol{a}_i^T}{||\boldsymbol{a}_i||^2} \right)^{\otimes 2} \right)$$

- Can be computed in $O(mn^2)$ time
- Must be positive; exponential convergence confirmed

1. Exact MSE formula and decay rate

2. **Optimization of row selection probabilities**

3. “Quenched error exponent”

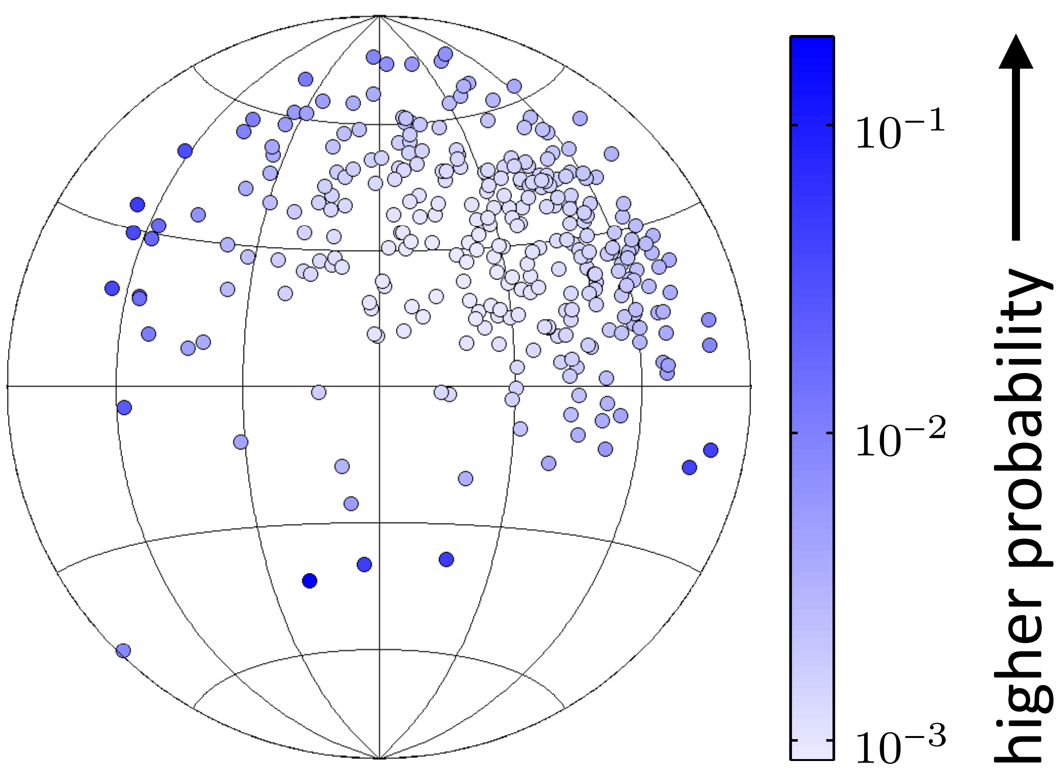
Optimal row selection

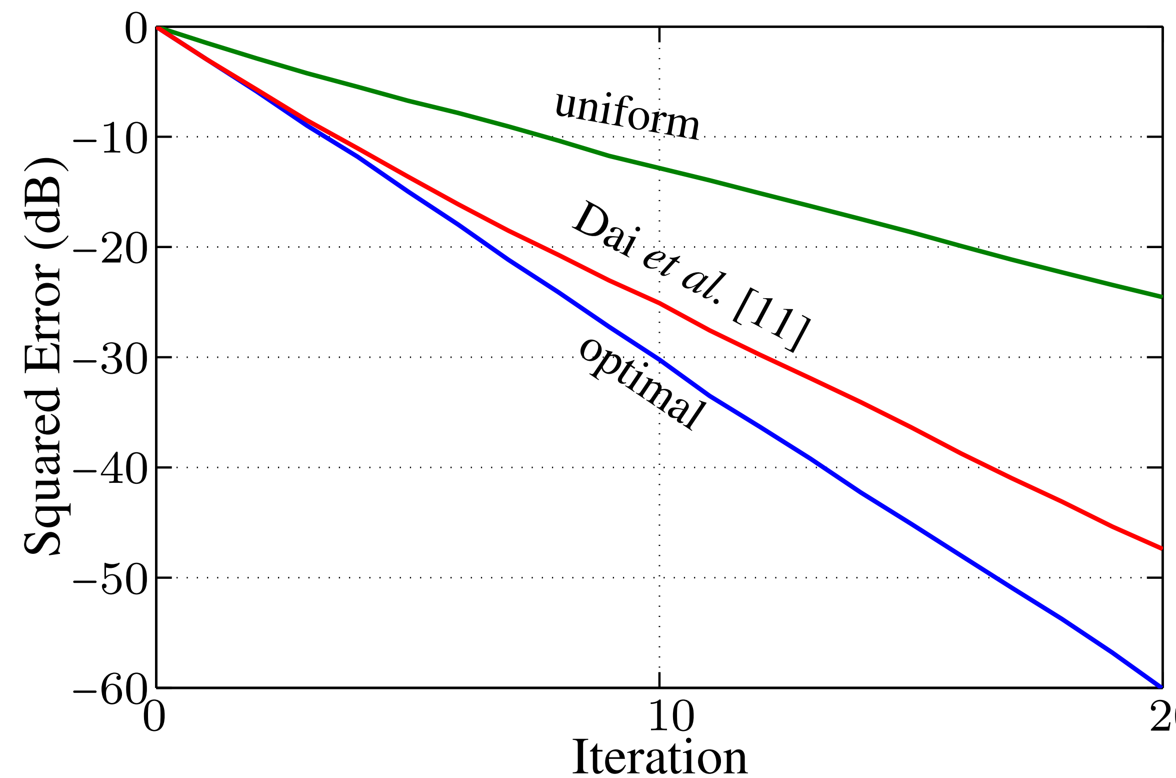
Convex optimization problem: minimize error exponent.

$$(p_1, \ldots, p_m) = \operatorname{argmin}_{\boldsymbol{p}} \lambda_{\max} \left(\sum_i p_i \left(\boldsymbol{I} - \frac{\boldsymbol{a}_i \boldsymbol{a}_i^T}{||\boldsymbol{a}_i||^2} \right)^{\otimes 2} \right)$$

semi-definite programming

n = 3 lets us easily visualize the optimal probabilities





Intuition: explorers of sparsely-populated regions chosen with higher probability

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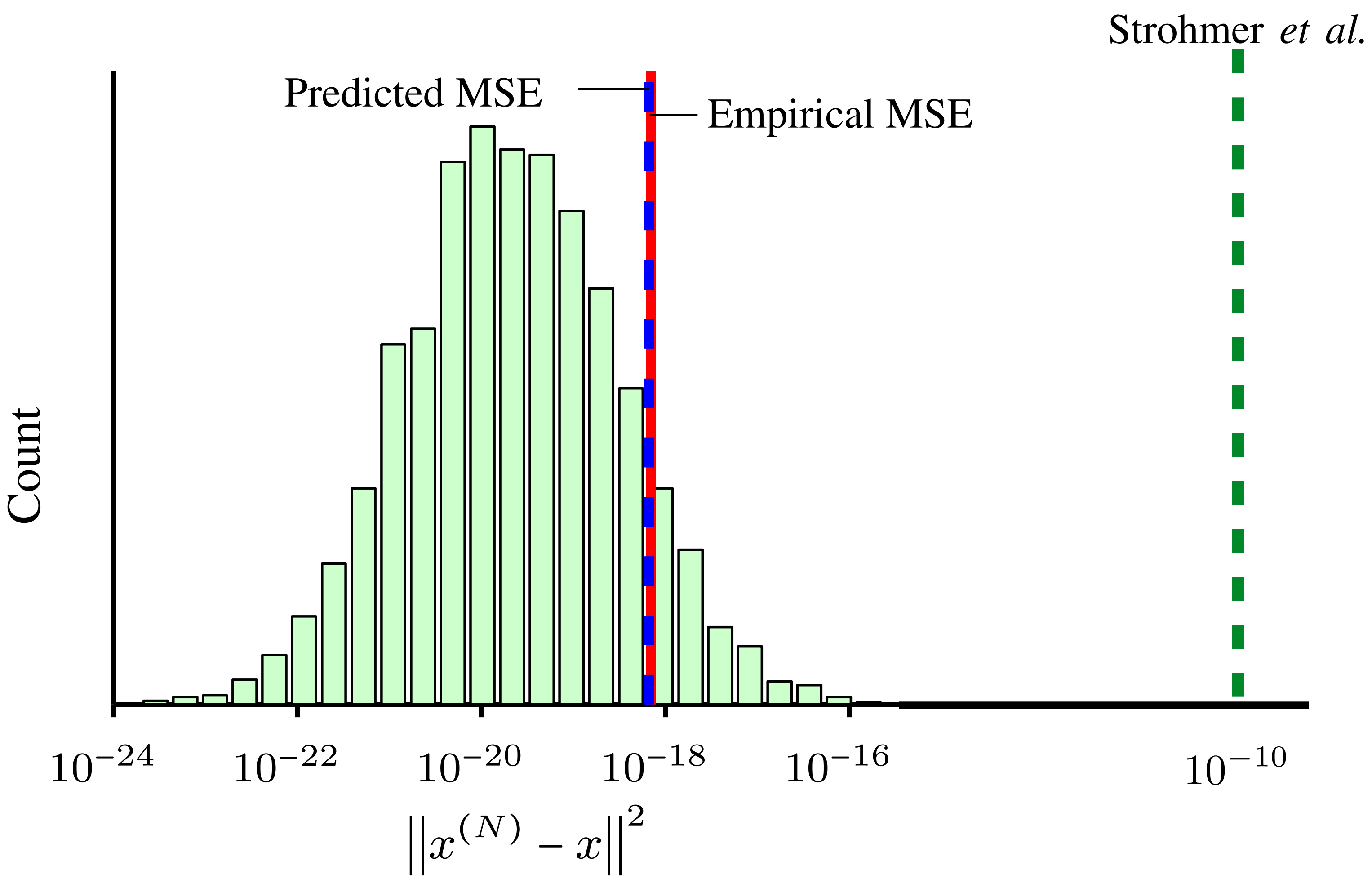
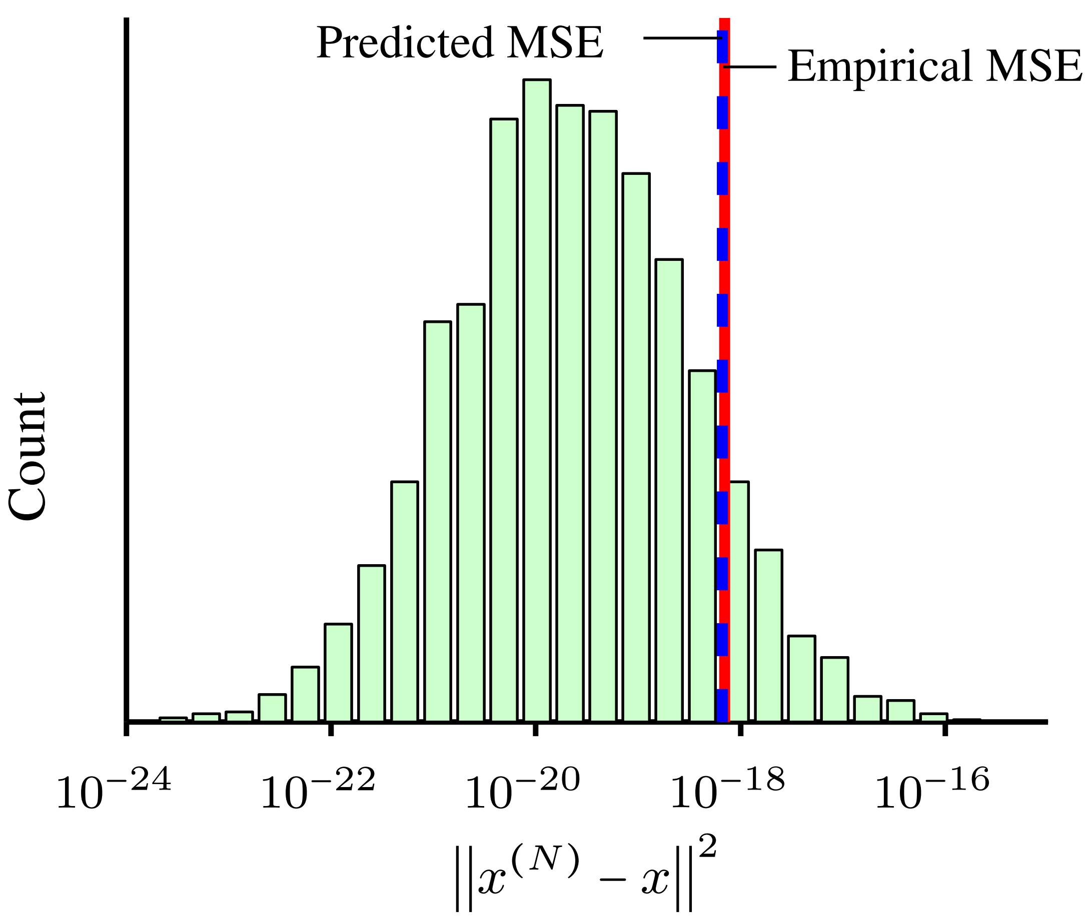
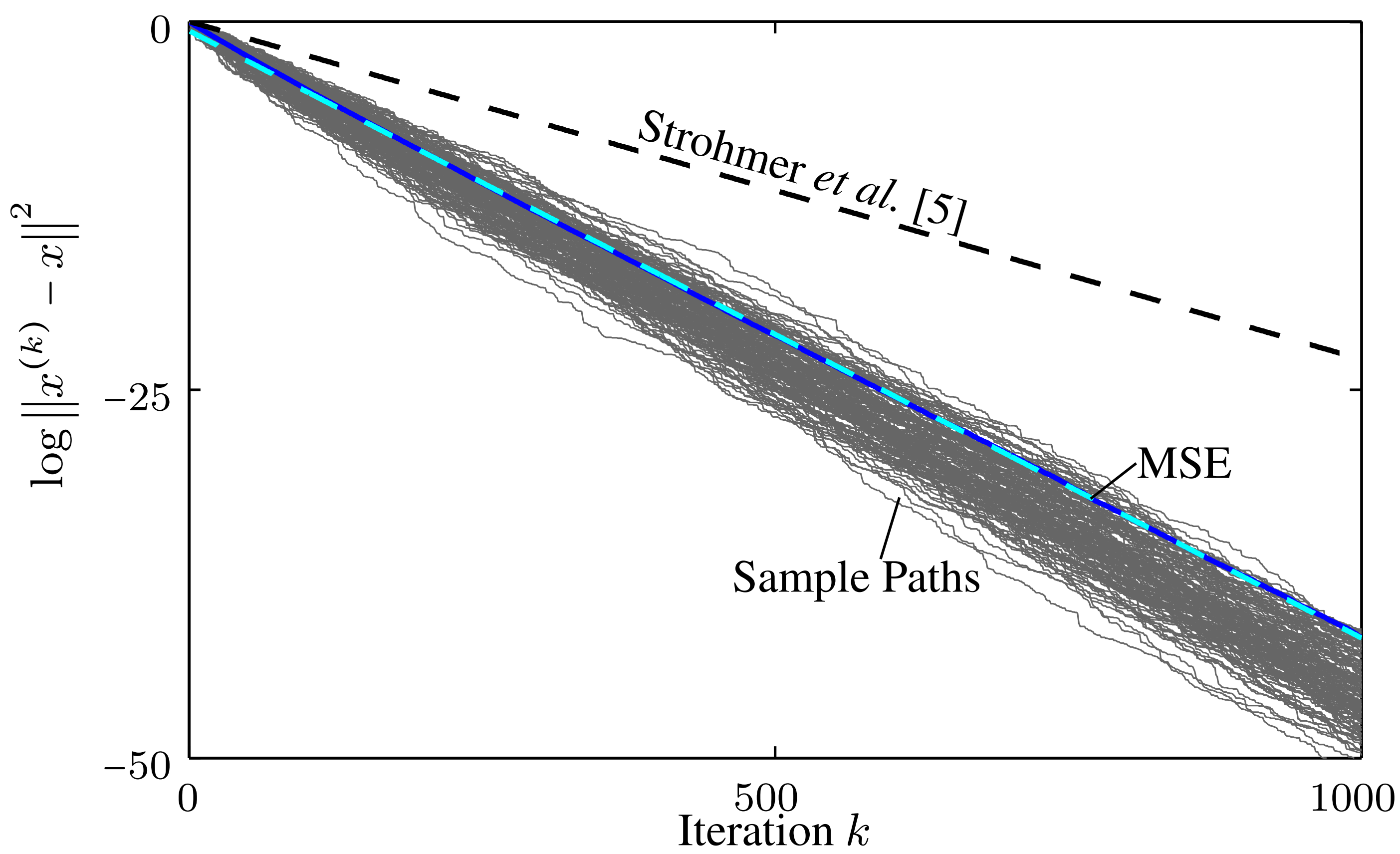


150 x 20 matrix w/ Gaussian entries.





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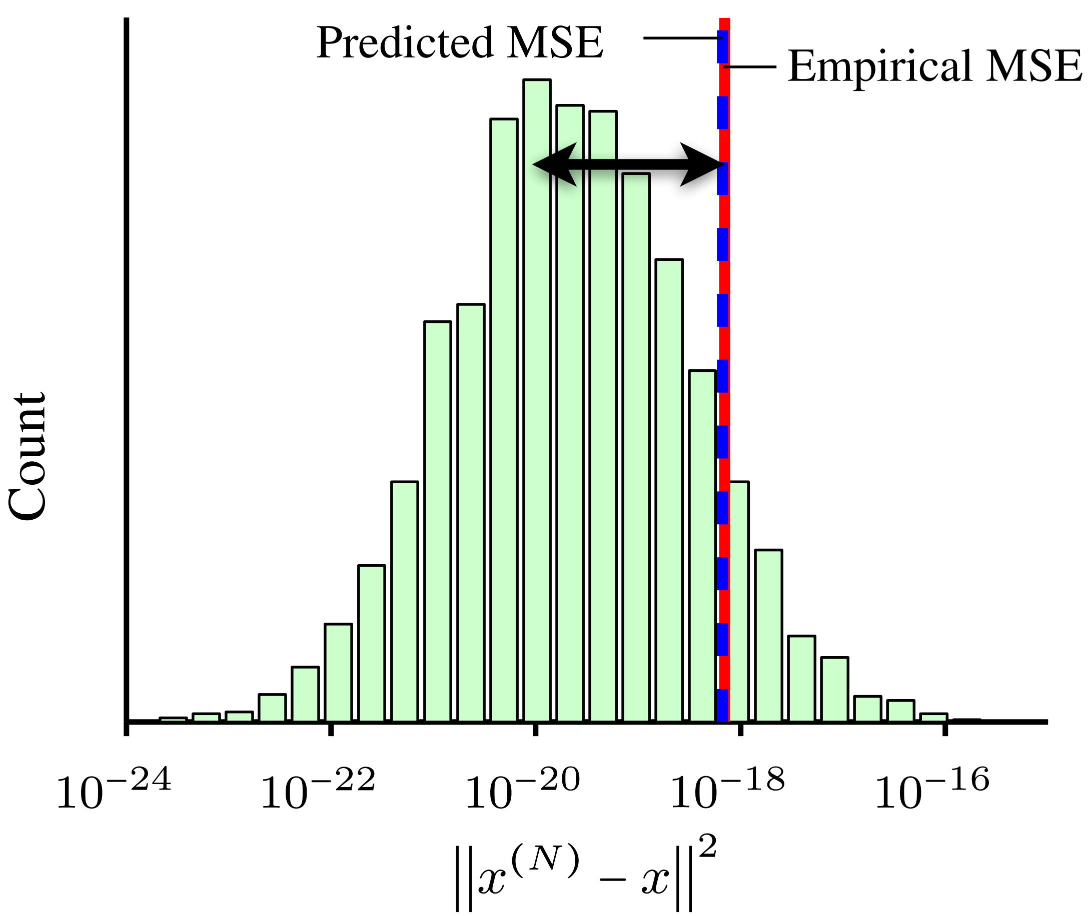
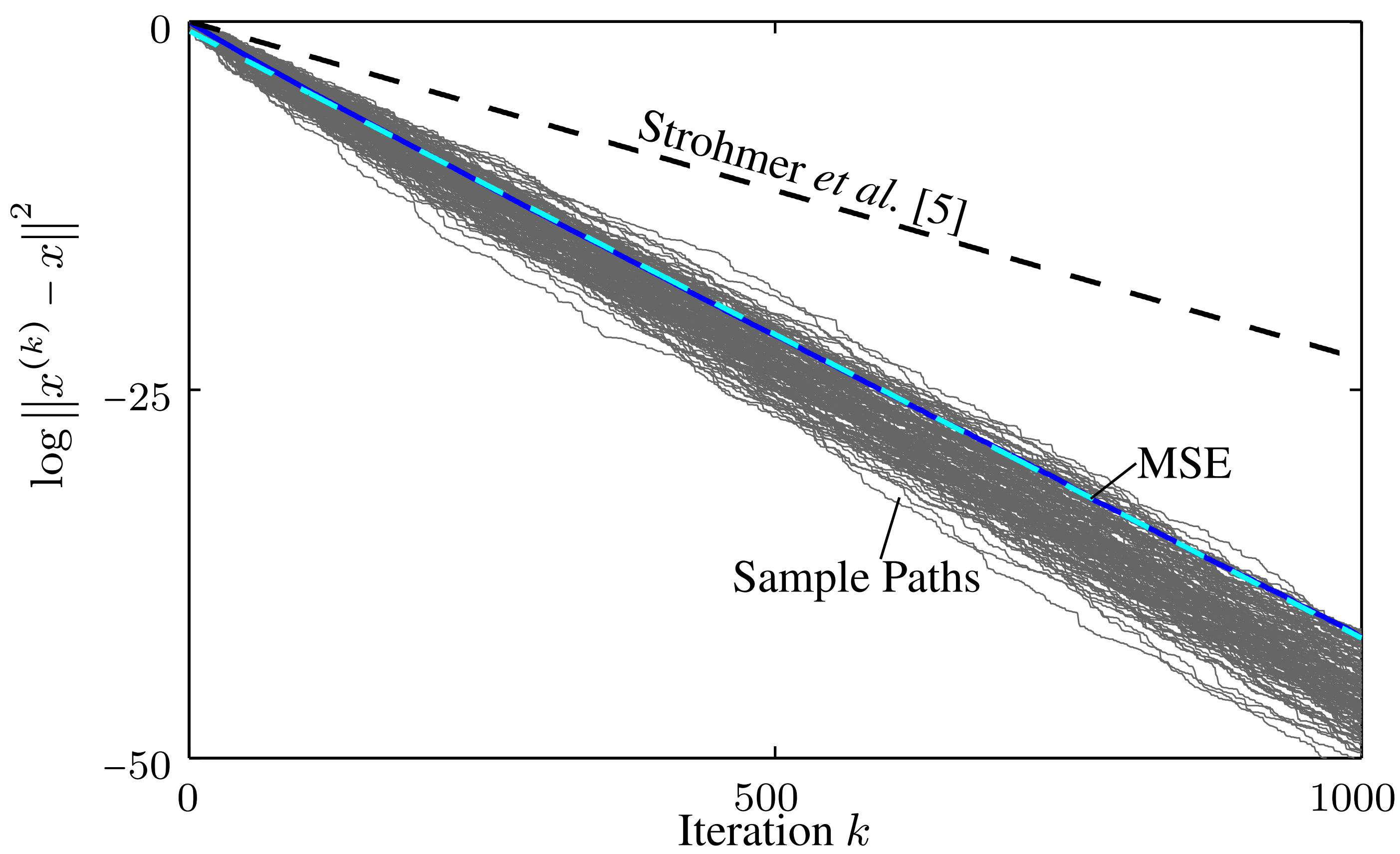
Simulations





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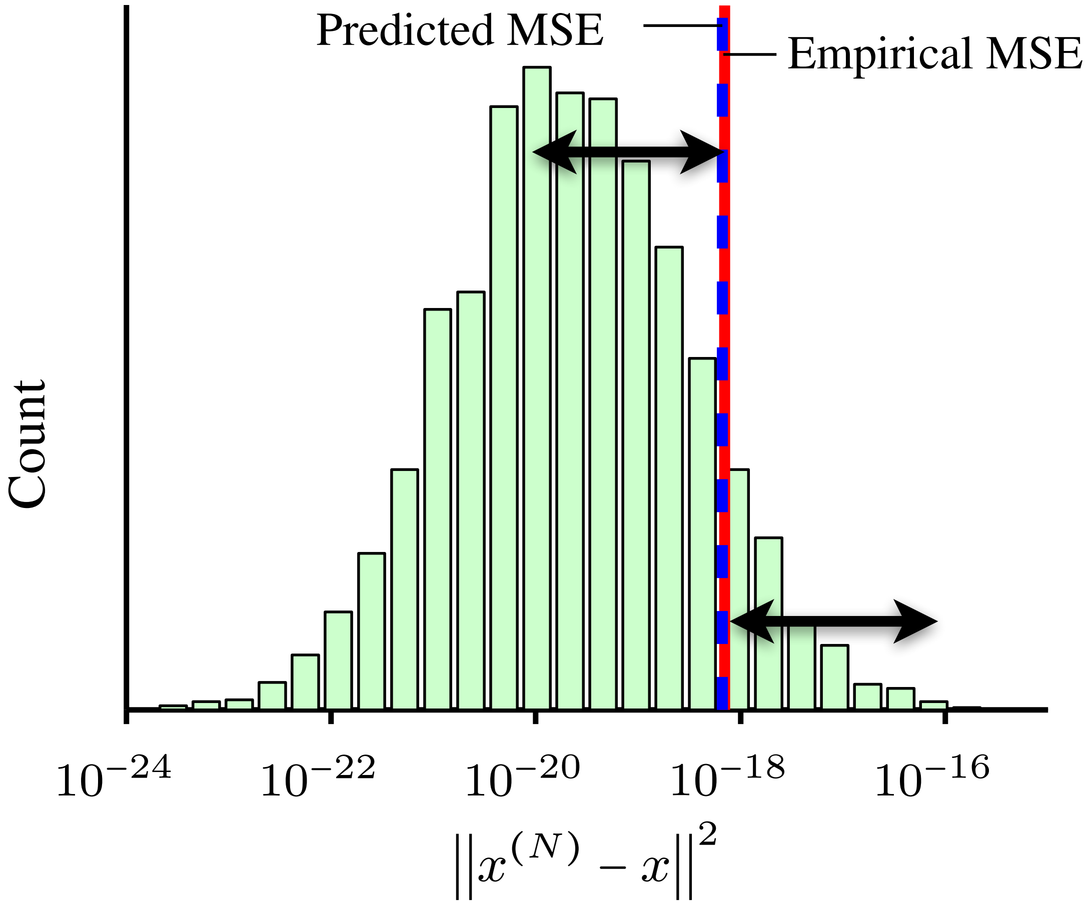
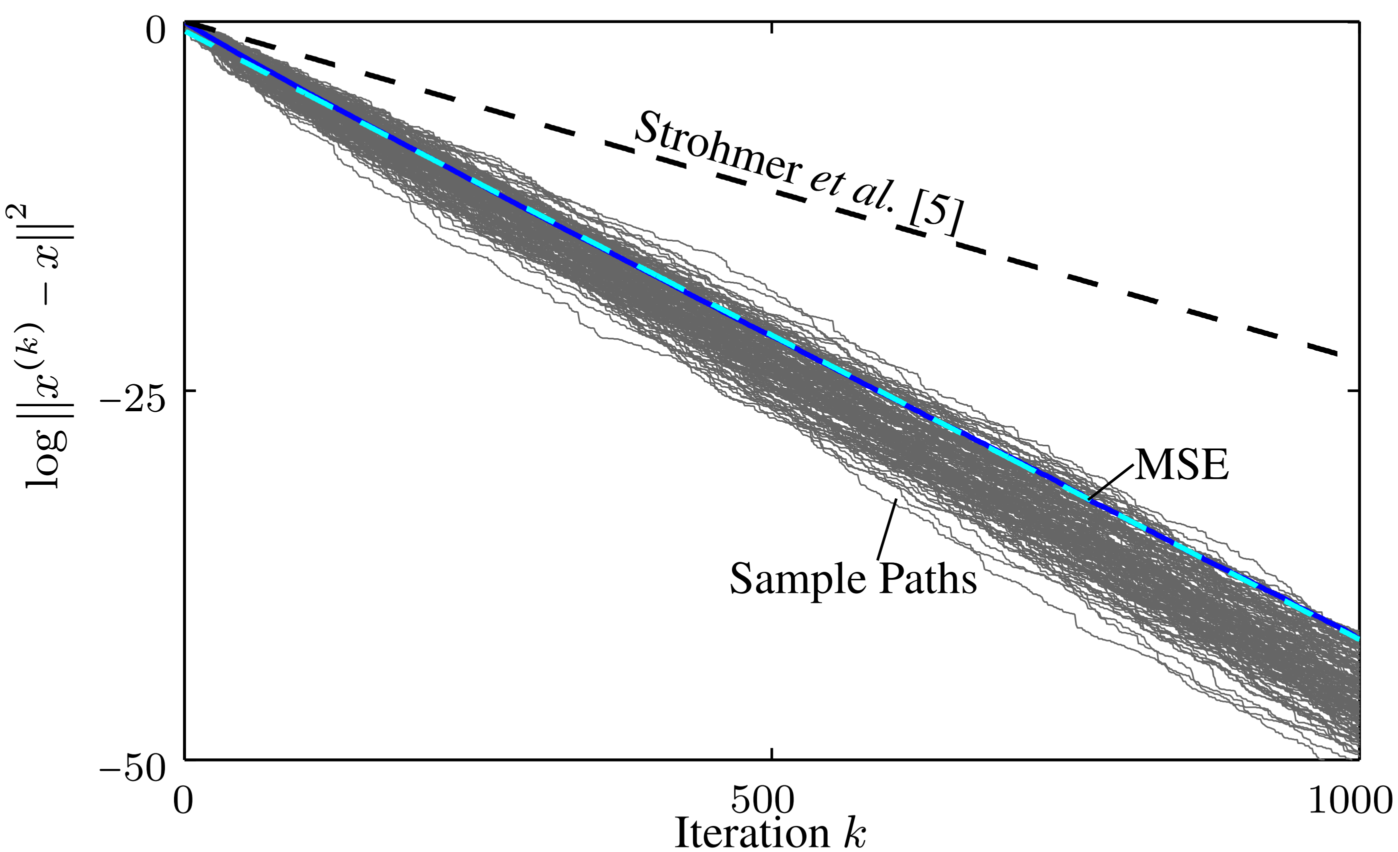




150 x 20 matrix w/ Gaussian entries.


IF YOU WANT TO MEASURE
TYPICAL PERFORMANCE
DON'T
USE the MSE!
quickmeme.com

Quenched error exponent

Average performance:

Annealed error exponent

$$\gamma_a \stackrel{\text{def}}{=} \lim_{N\to\infty} -\frac{1}{N} \log \mathbb{E}||\boldsymbol{z}^{(N)}||^2$$

Typical performance:

Quenched error exponent

$$\gamma_q \stackrel{\text{def}}{=} \lim_{N\to\infty} -\frac{1}{N} \mathbb{E} \log ||\boldsymbol{z}^{(N)}||^2$$

- Much more difficult to analyze.
- Known to physicists as the top ***Lyapunov exponent***.
- They use heuristics to solve.

Physicists have their own intuition for this trick, but we can get the same result by assuming the error is log-normal:

Assume

$$\log ||\boldsymbol{z}^{(N)}||^2 \sim \mathcal{N}(N\mu, N\sigma^2).$$

Then

$$\gamma_q = -\mu$$

$$\mathbb{E}||\boldsymbol{z}^{(N)}||^2 = \exp(N[\mu + \frac{1}{2}\sigma^2])$$

$$\mathbb{E}||\boldsymbol{z}^{(N)}||^4 = \exp(N[2\mu + 2\sigma^2])$$

Naive replica method $\log Z = \lim_{n \to 0} \frac{Z^n - 1}{n}$

Solve

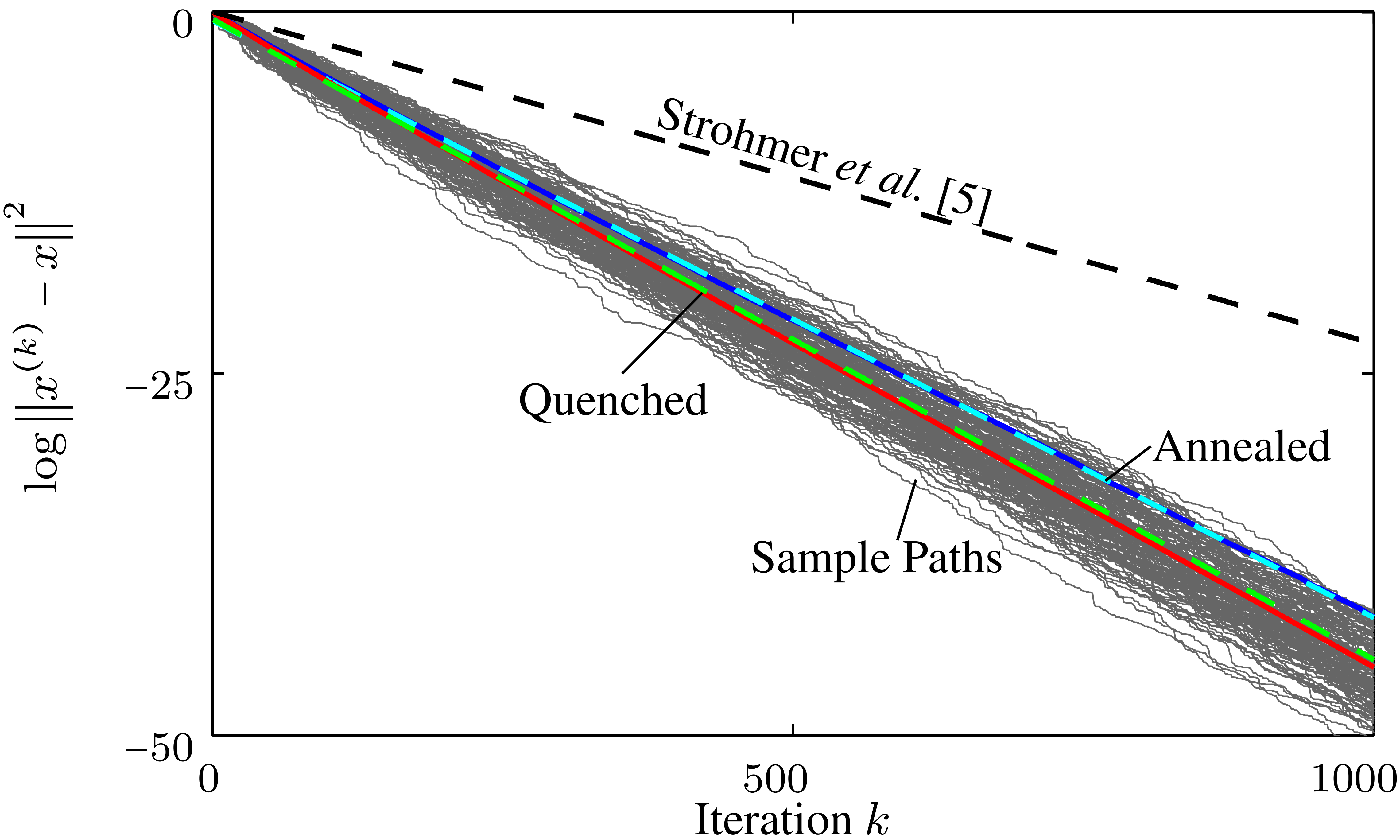
$$\mu = \frac{1}{N}\left[2\log\mathbb{E}||\boldsymbol{z}^{(N)}||^2 - \frac{1}{2}\log\mathbb{E}||\boldsymbol{z}^{(N)}||^4\right]$$

$$\gamma_q \approx 2\gamma_a - \frac{1}{2}\gamma_a^{(2)}$$

where $\gamma_a^{(2)} = -\log\lambda_{\max}\left(\sum_i p_i\left(\boldsymbol{I} - \frac{\boldsymbol{a}_i\boldsymbol{a}_i^T}{||\boldsymbol{a}_i||^2}\right)^{\otimes 4}\right)$

Quenched error exponent

$$\gamma_q \stackrel{\text{def}}{=} \lim_{N\to\infty} -\frac{1}{N}\mathbb{E}\log||\boldsymbol{z}^{(N)}||^2$$



0
−25
−50
0
500
1000
Iteration k
$\log \|x^{(k)} - x\|^2$
Strohmer *et al.* [5]
Quenched
Annealed
Sample Paths

Summary

- ***Exact MSE formula for randomized Kaczmarz algorithms (and its generalizations)***

  Lifting!

- ***Annealed and quenched error exponents give decay rate***

  Average vs. typical performance

- ***Finding optimal row selection probabilities***

  Convex optimization