Deep Learning Book

Capítulo 2 - Álgebra Linear

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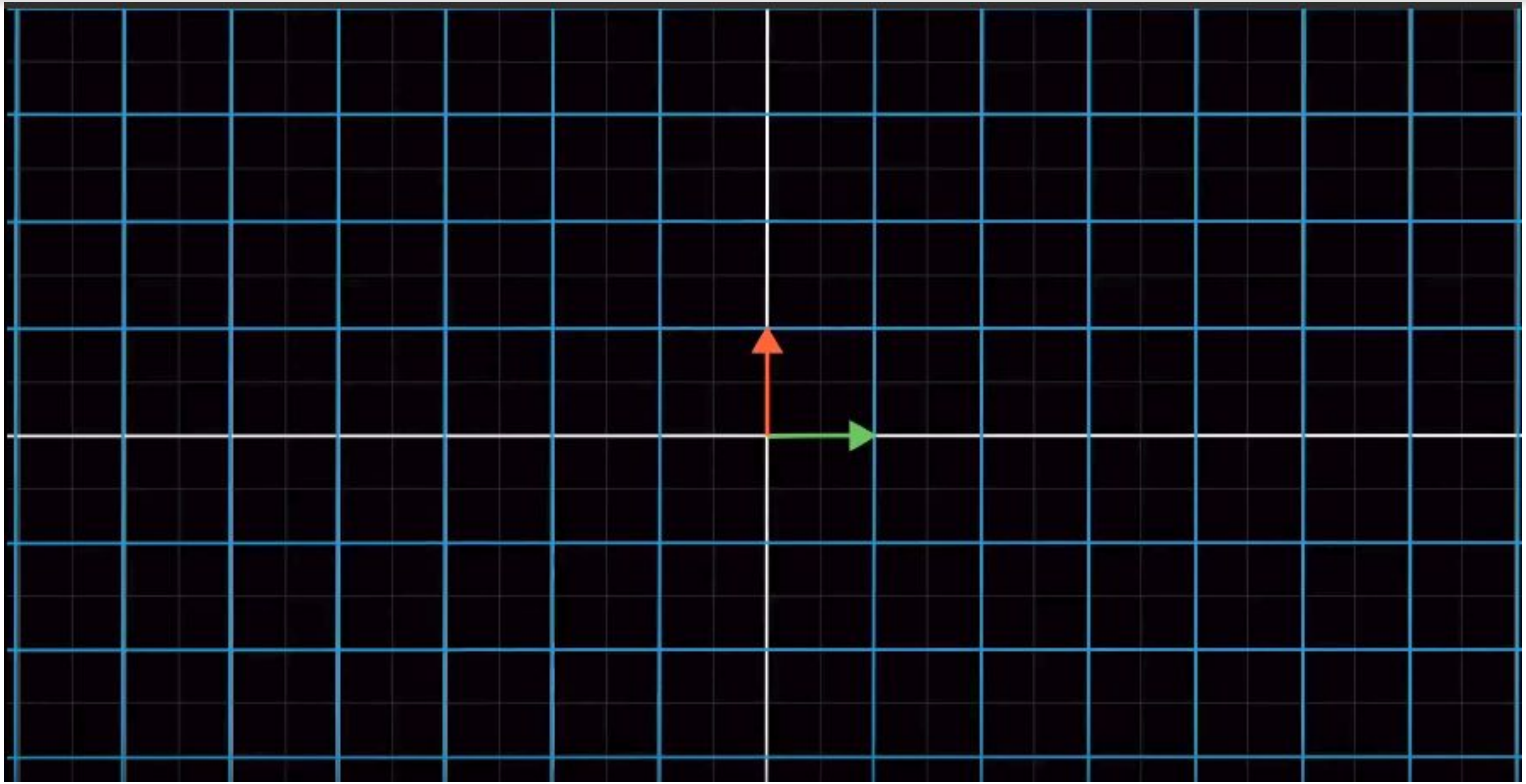
Autodecomposição



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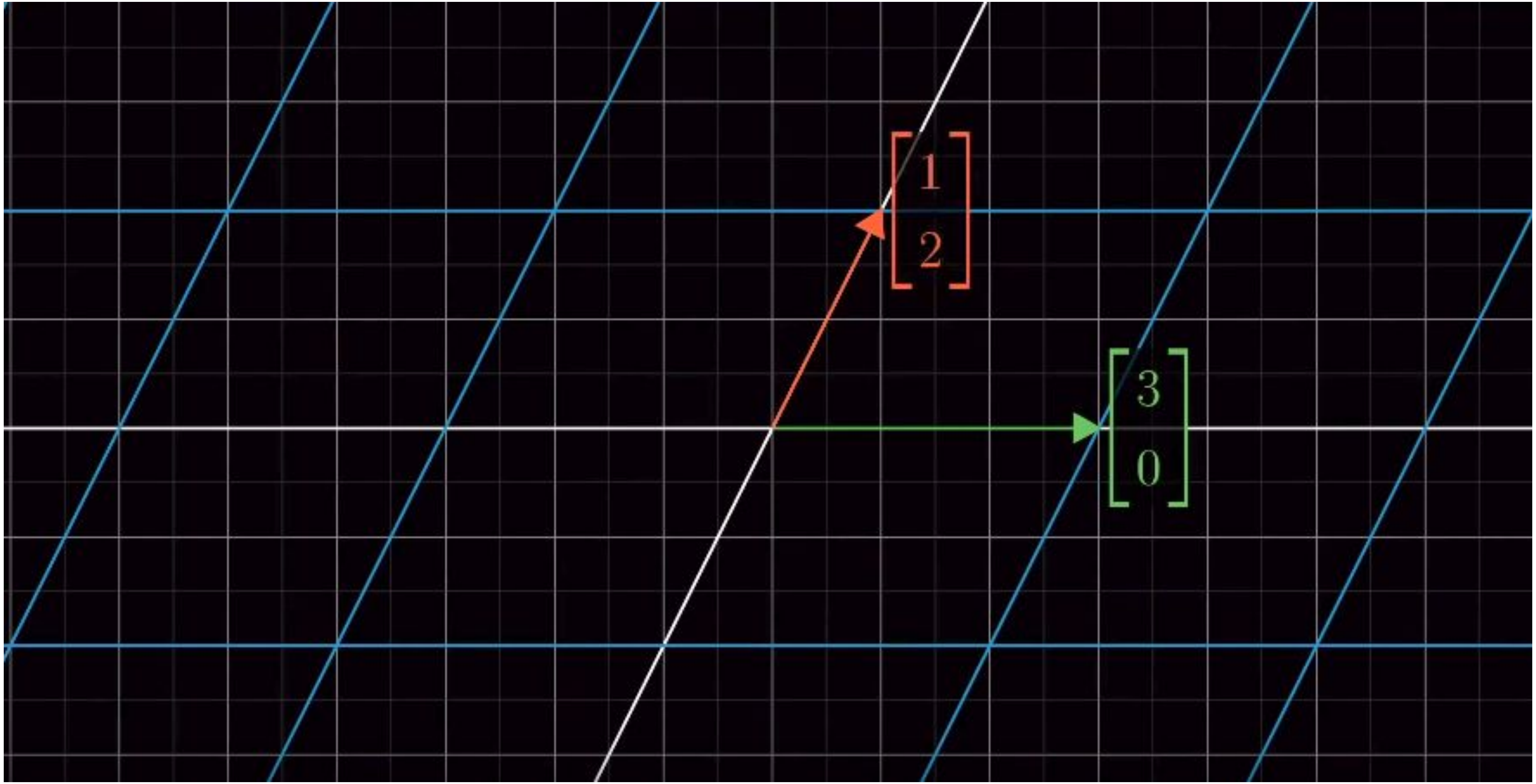

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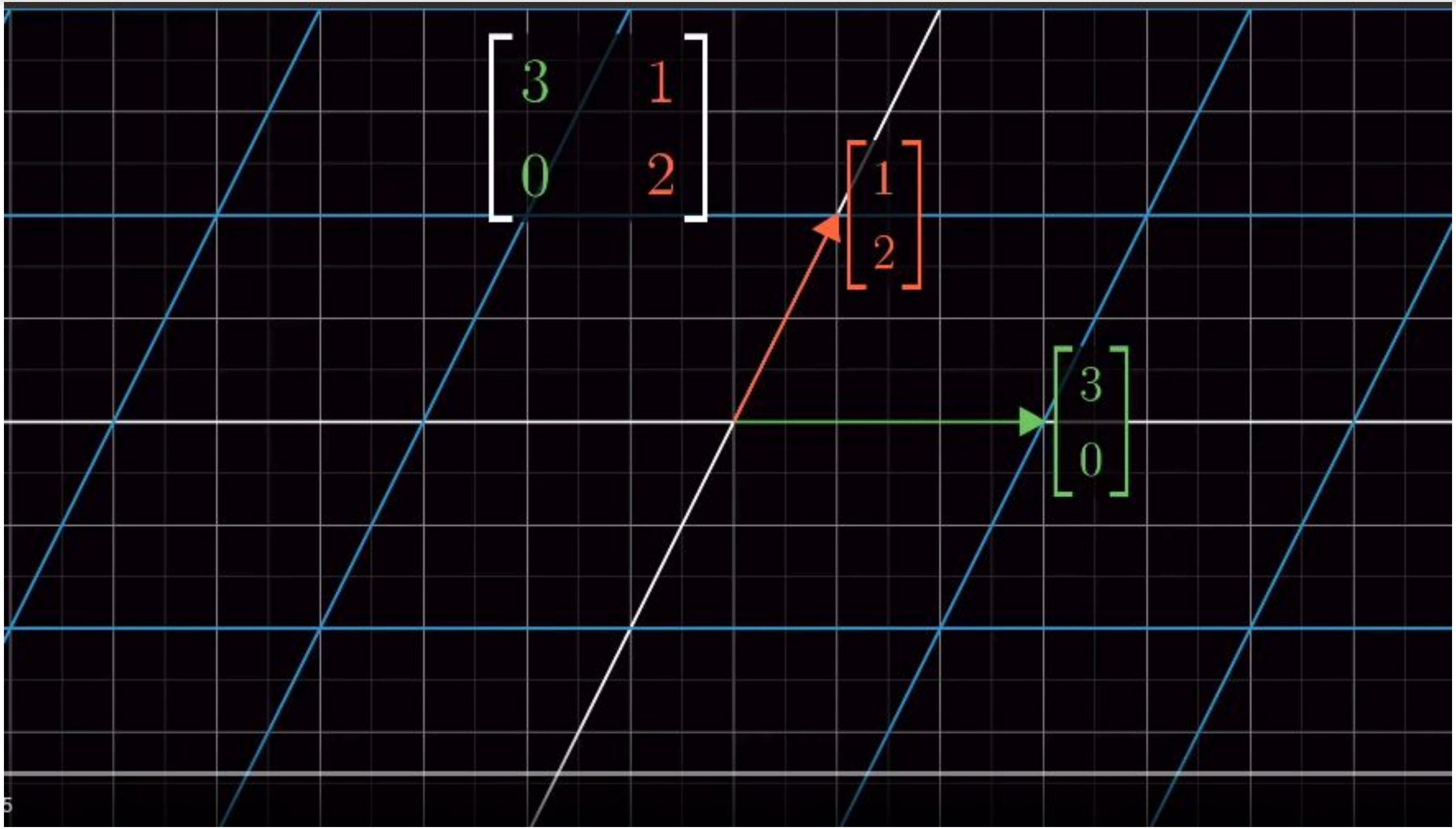

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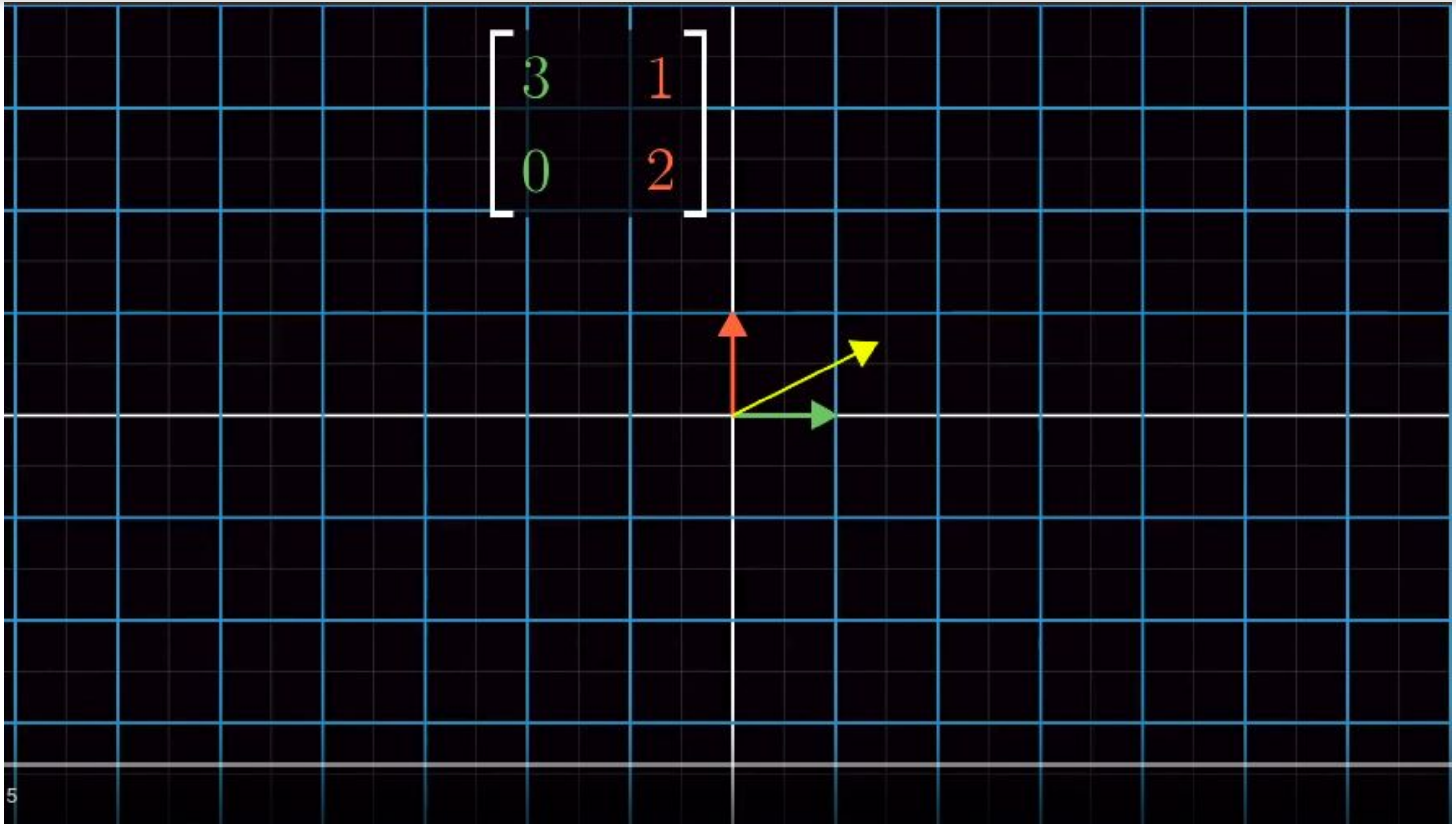

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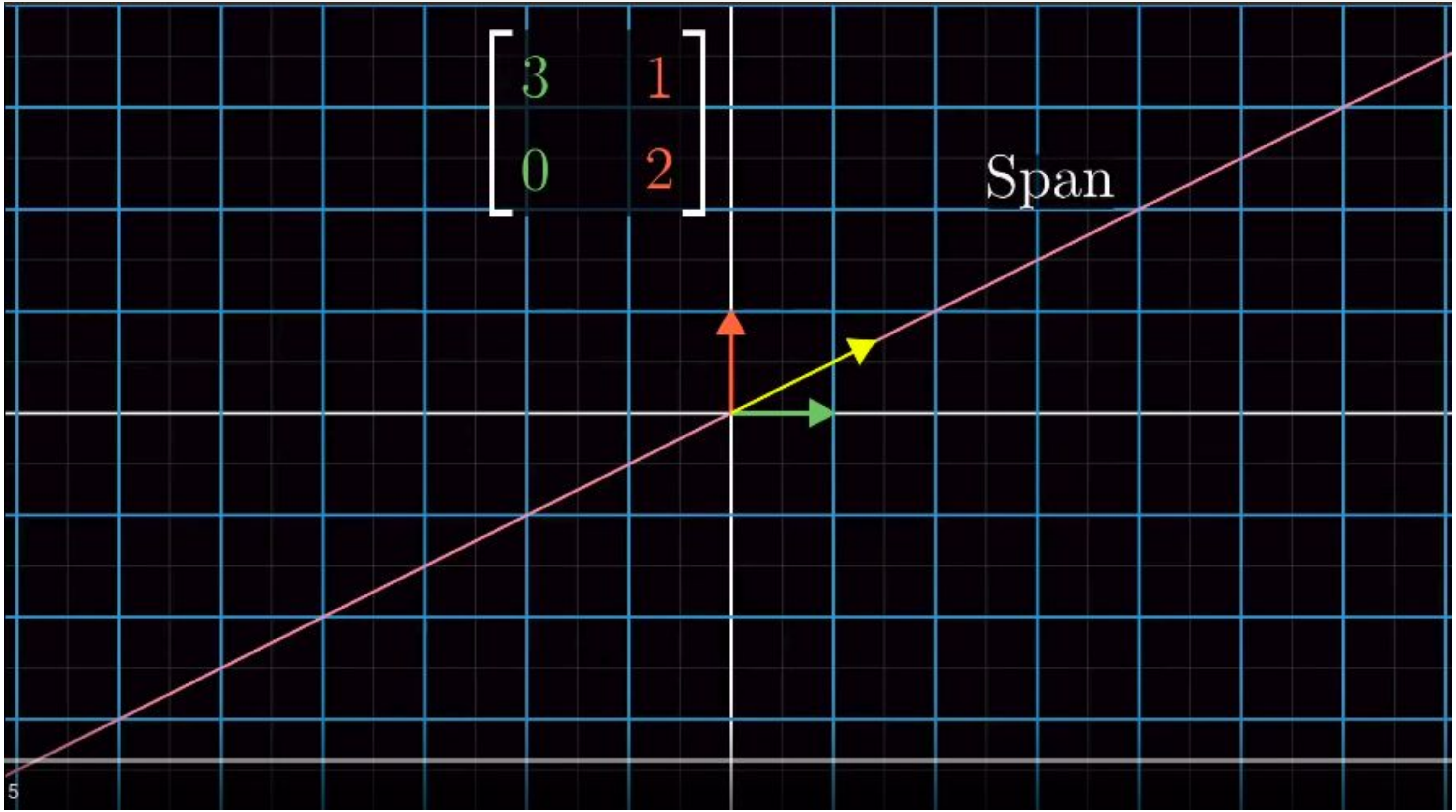

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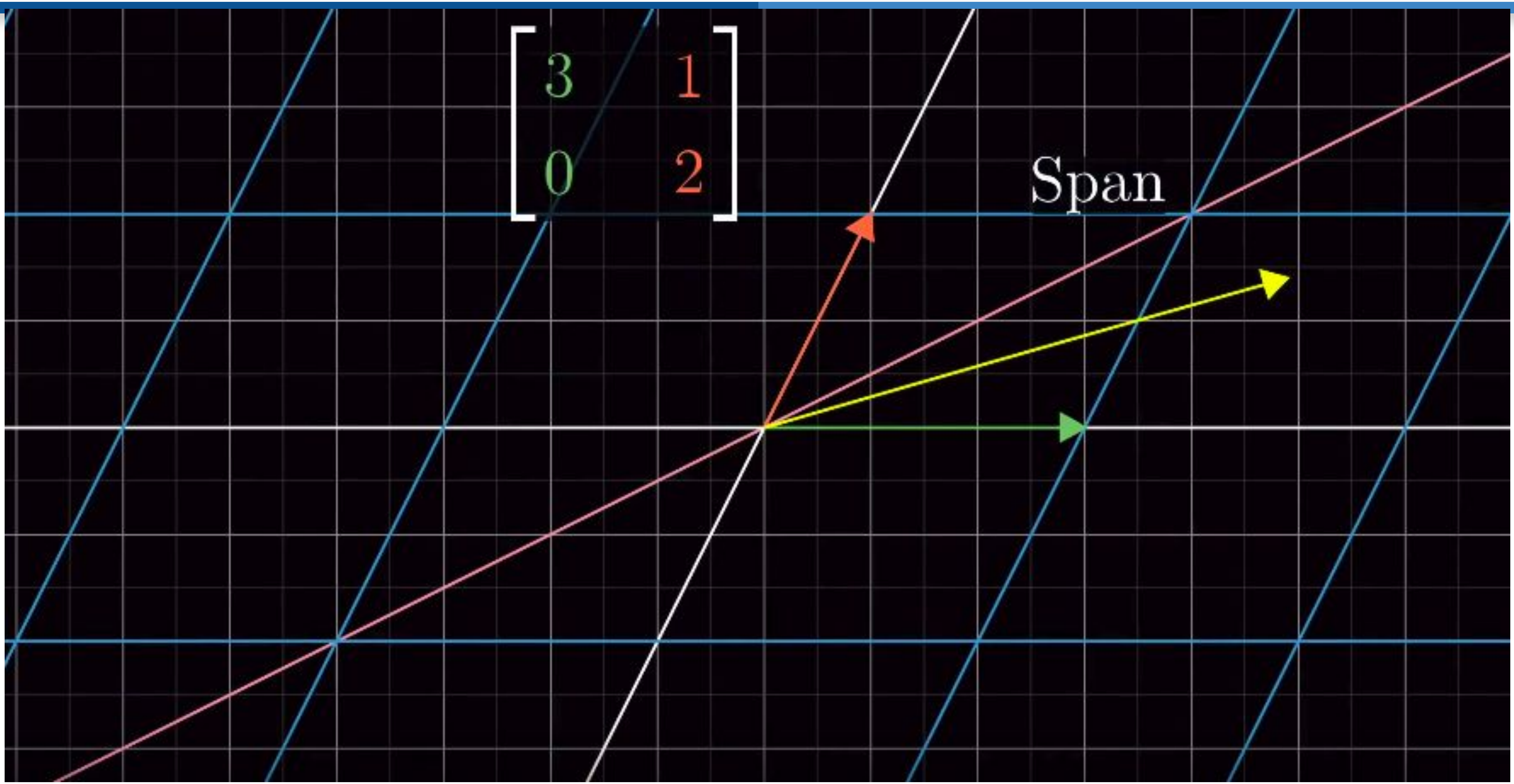

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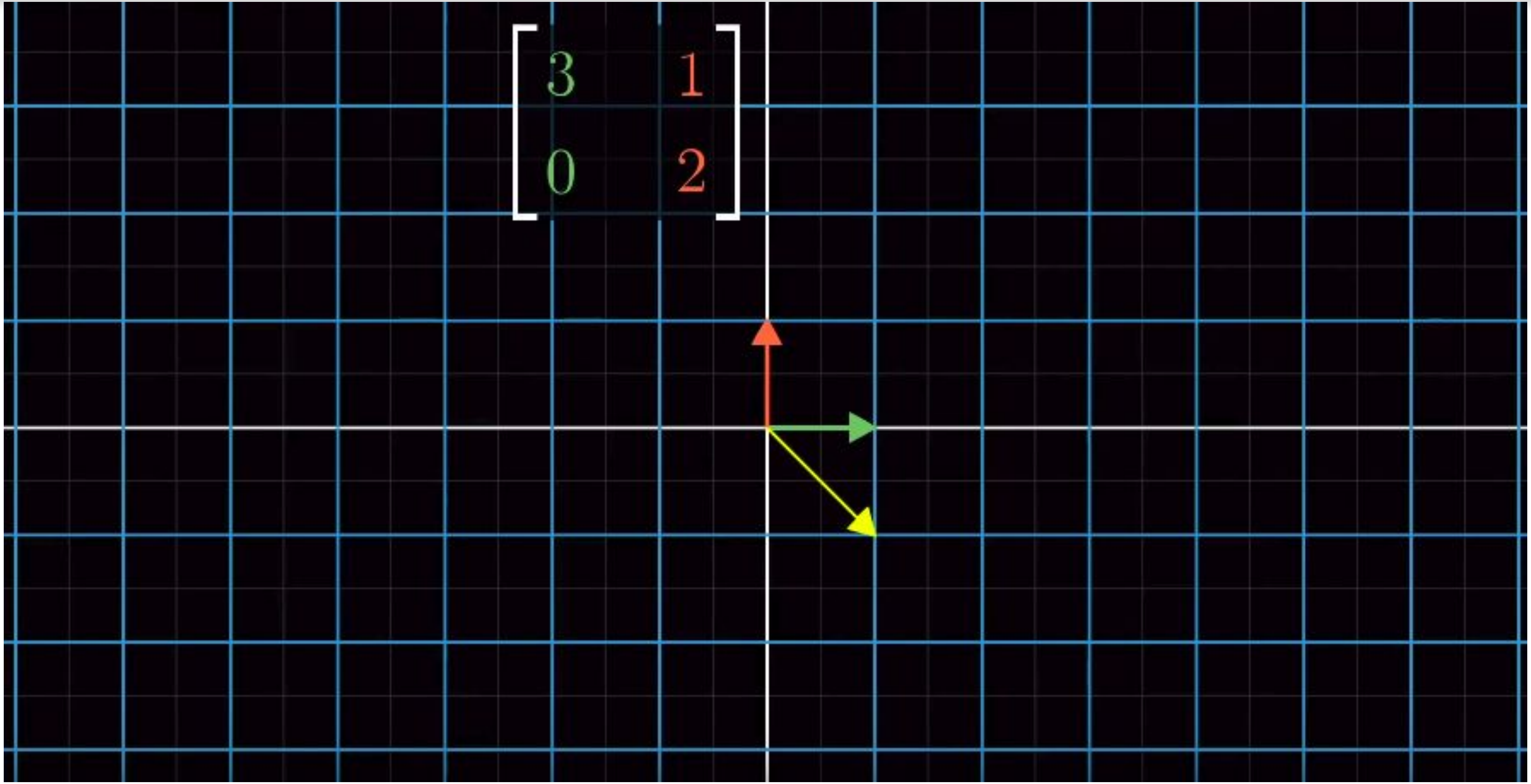

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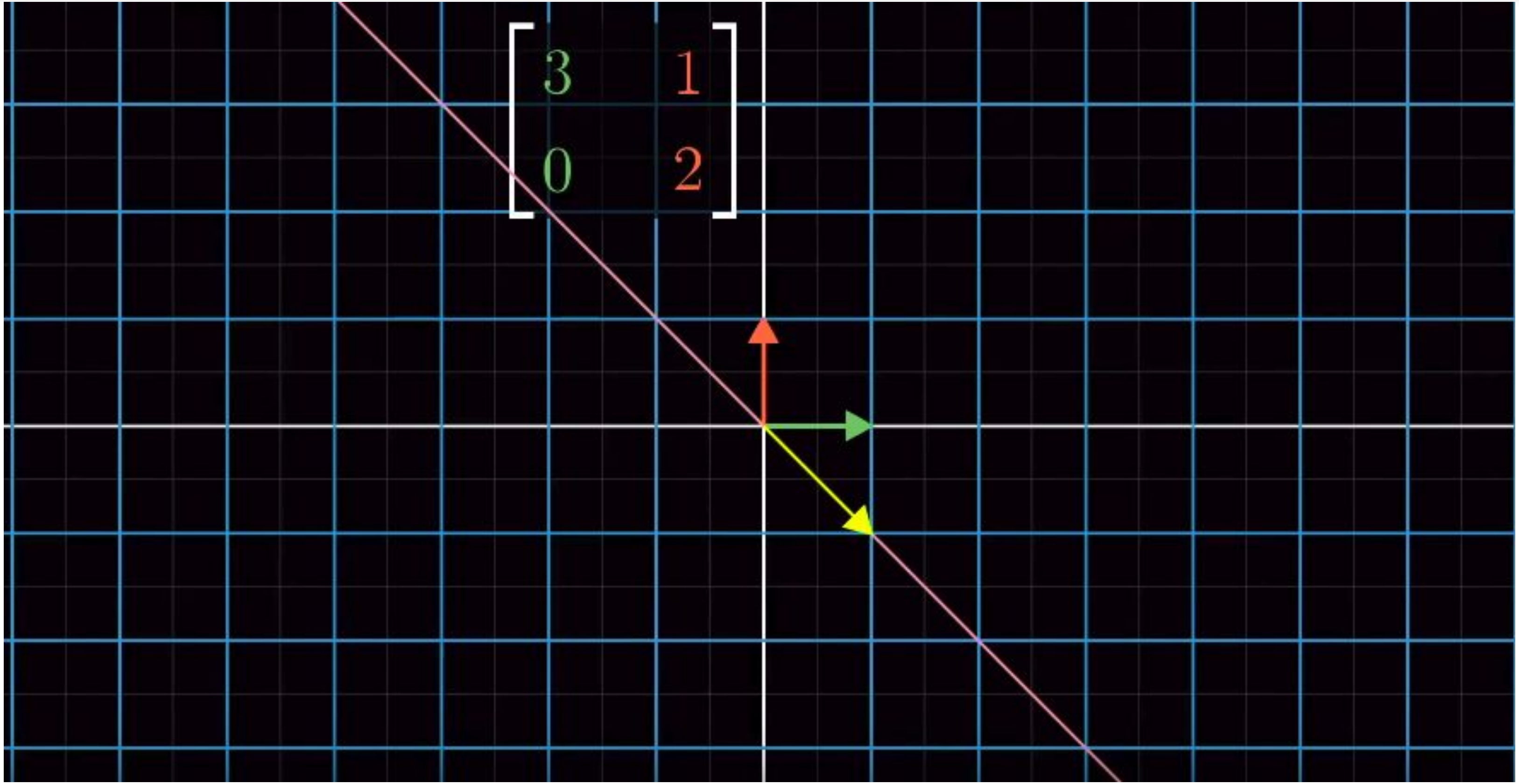

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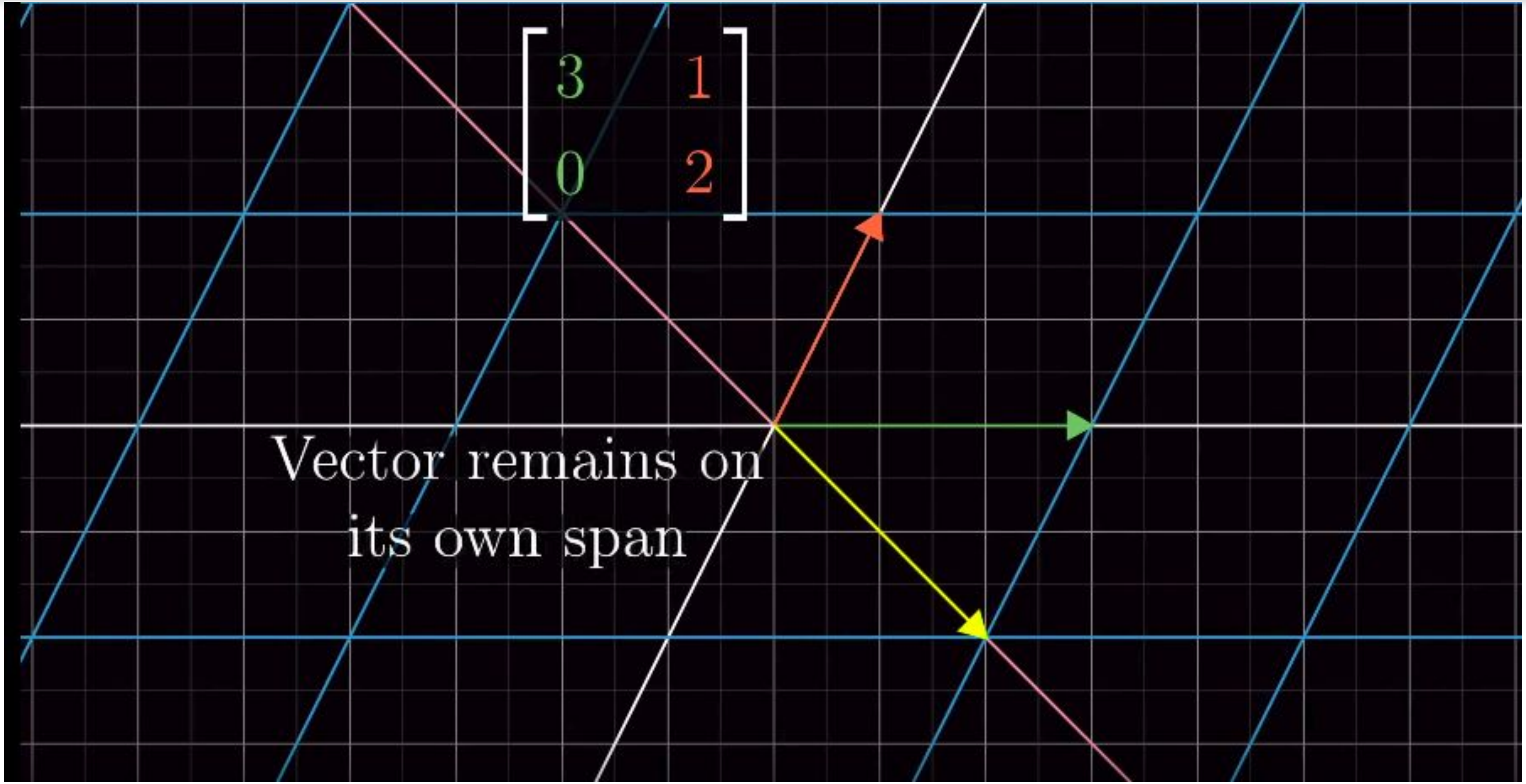

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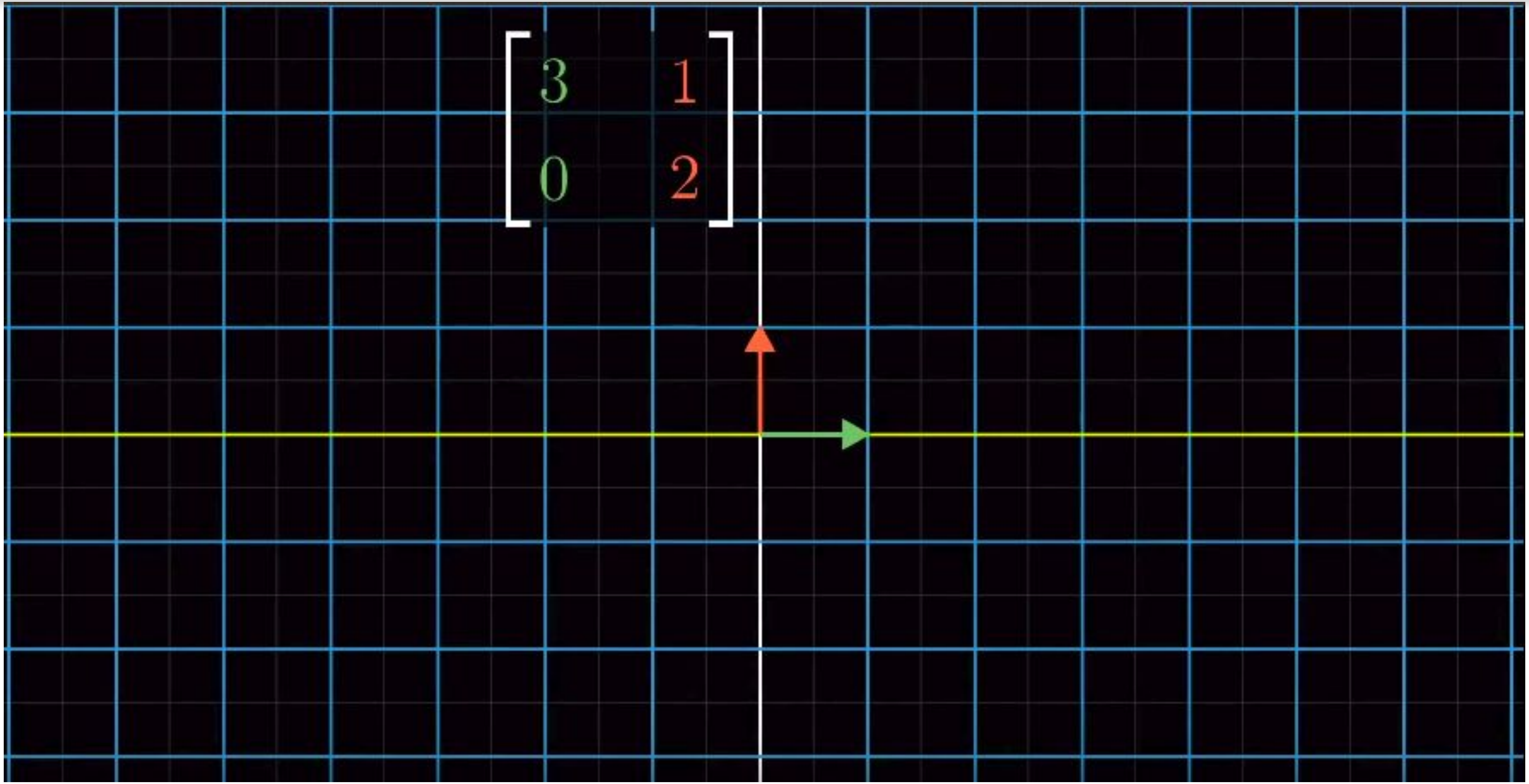

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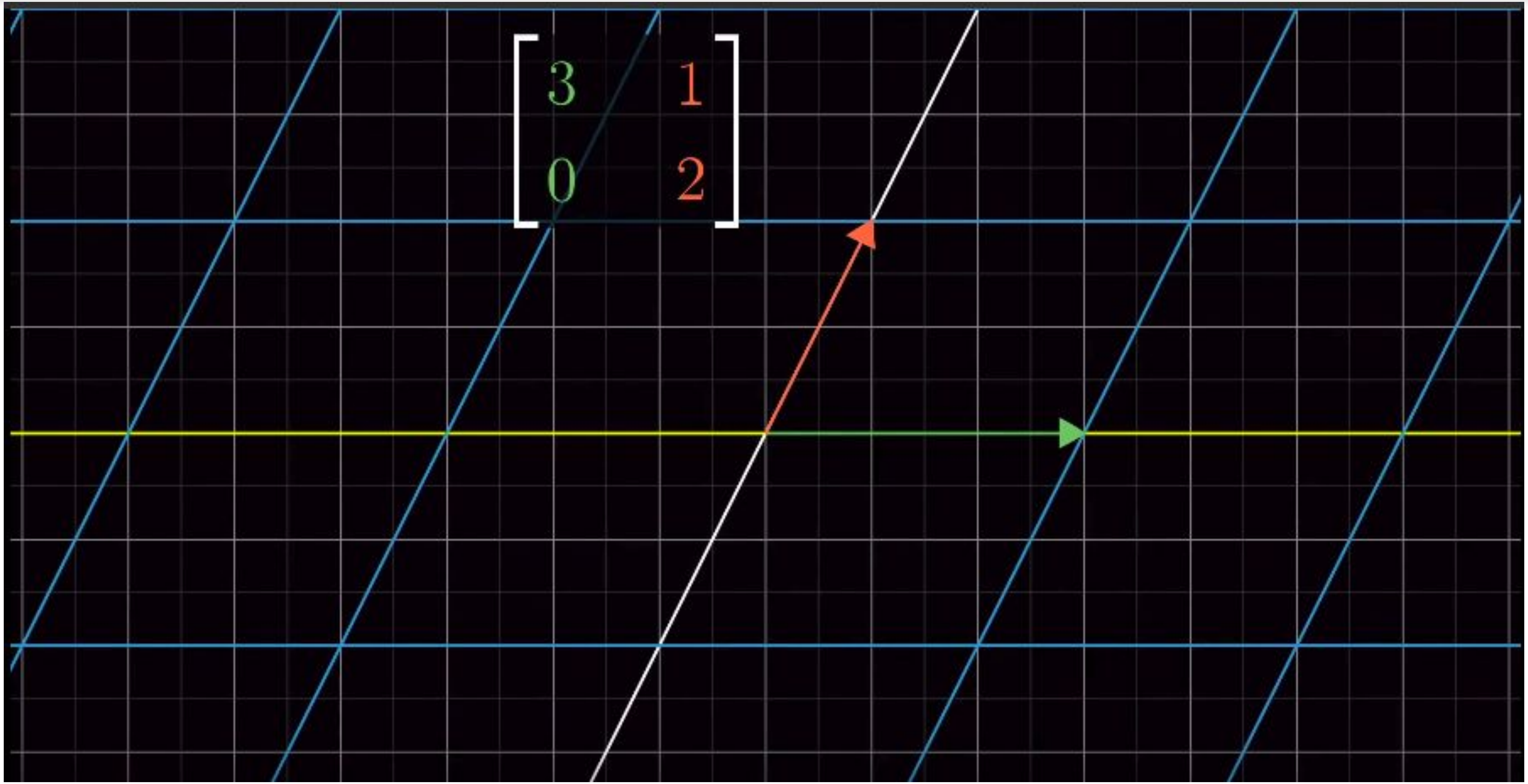

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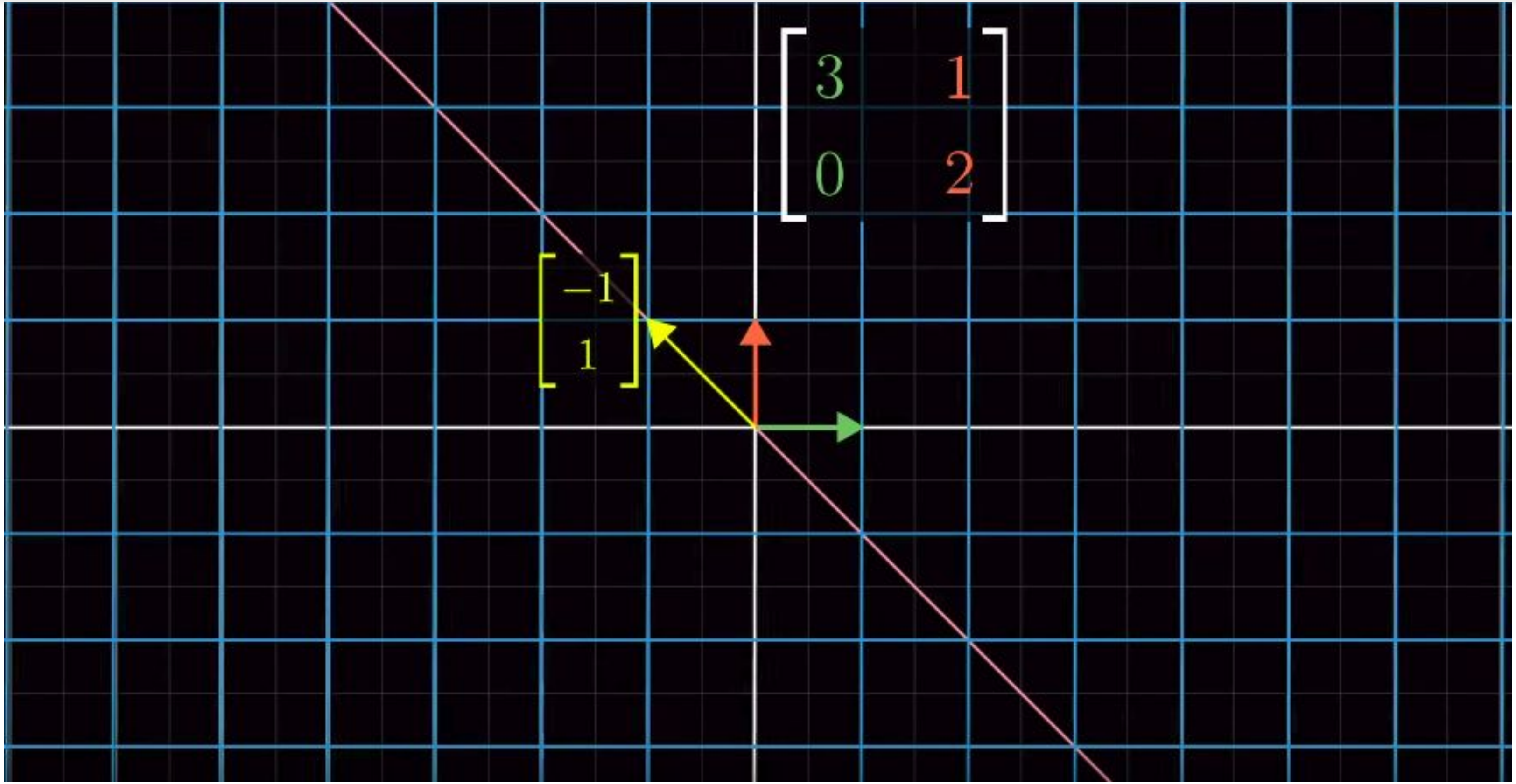

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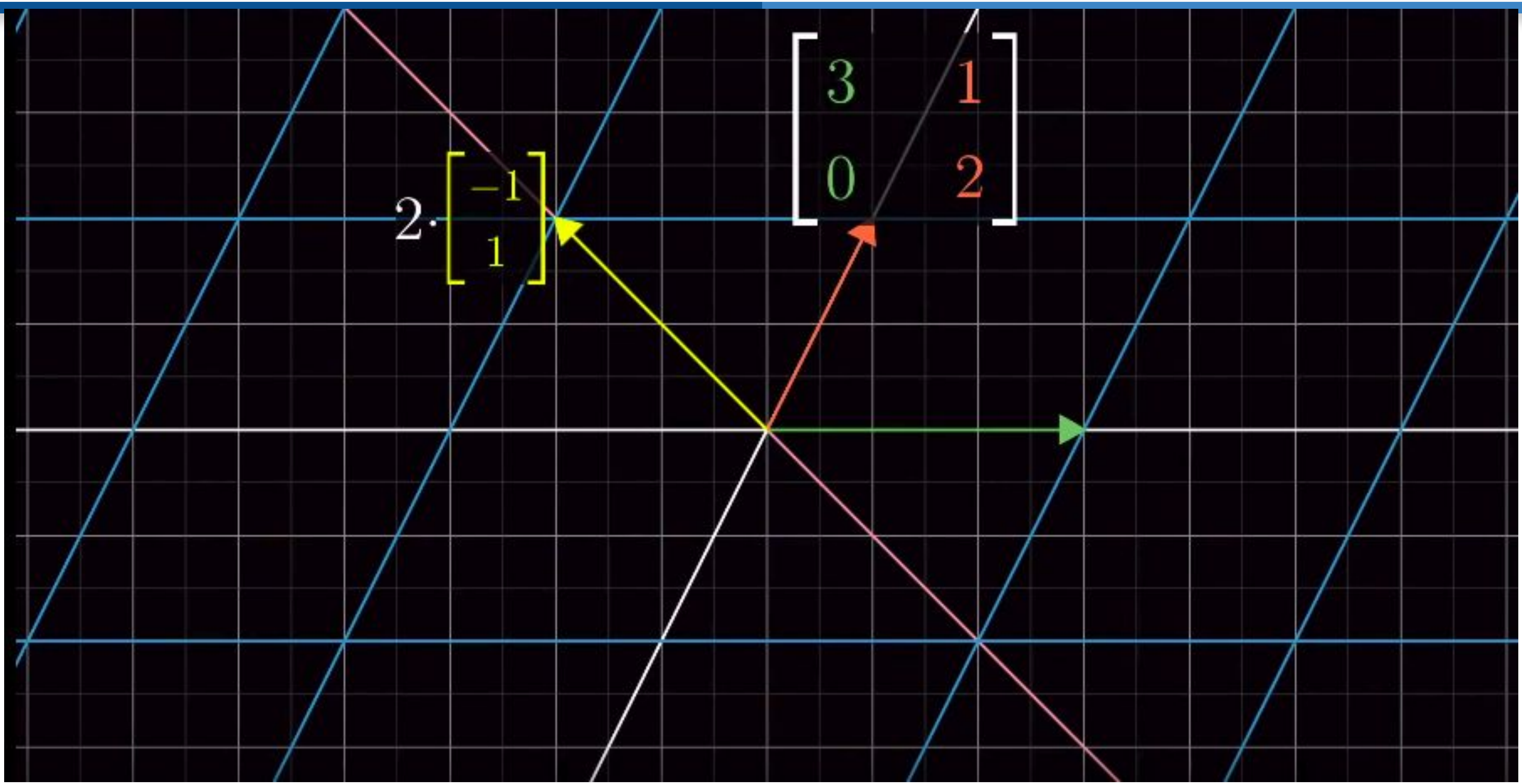

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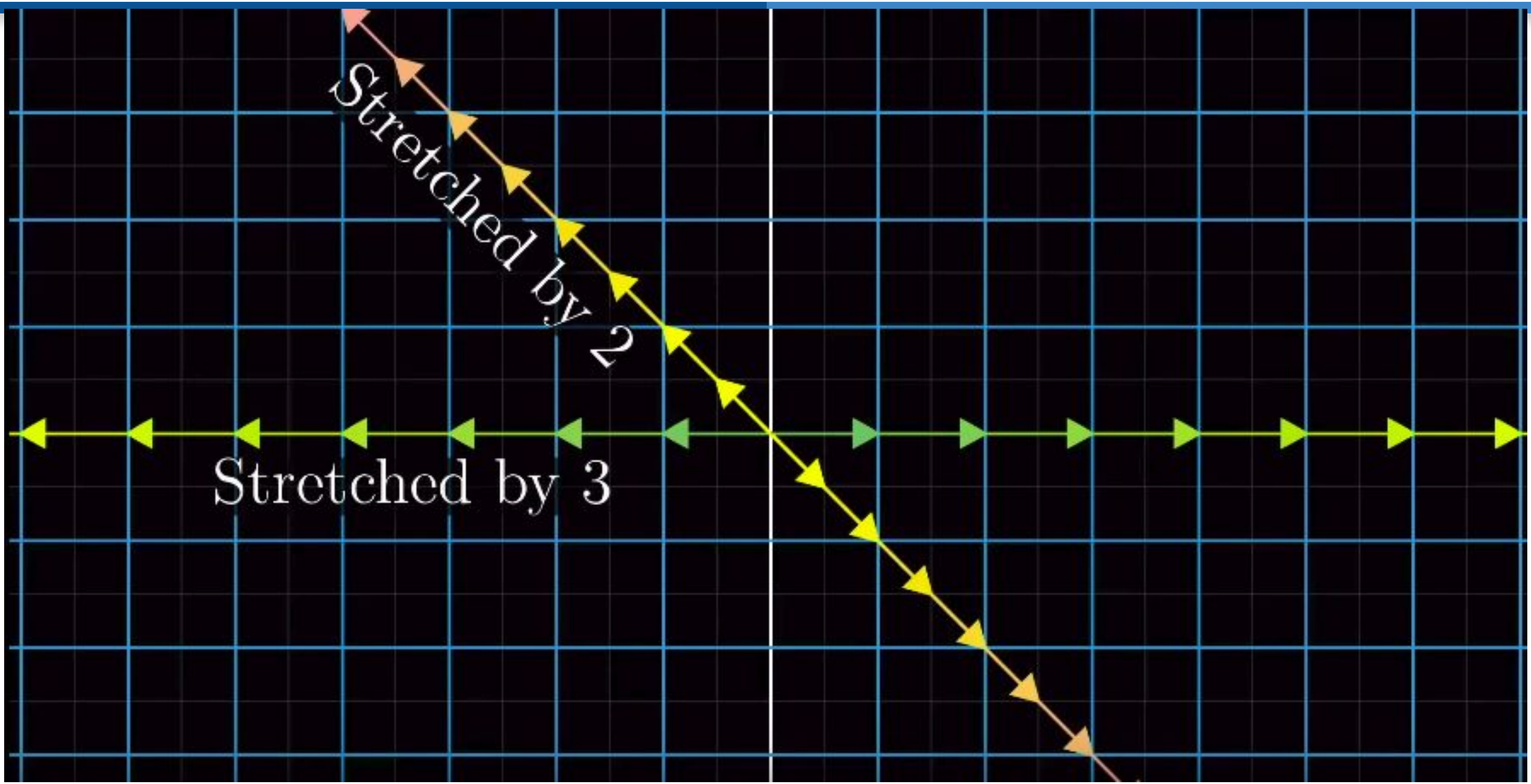

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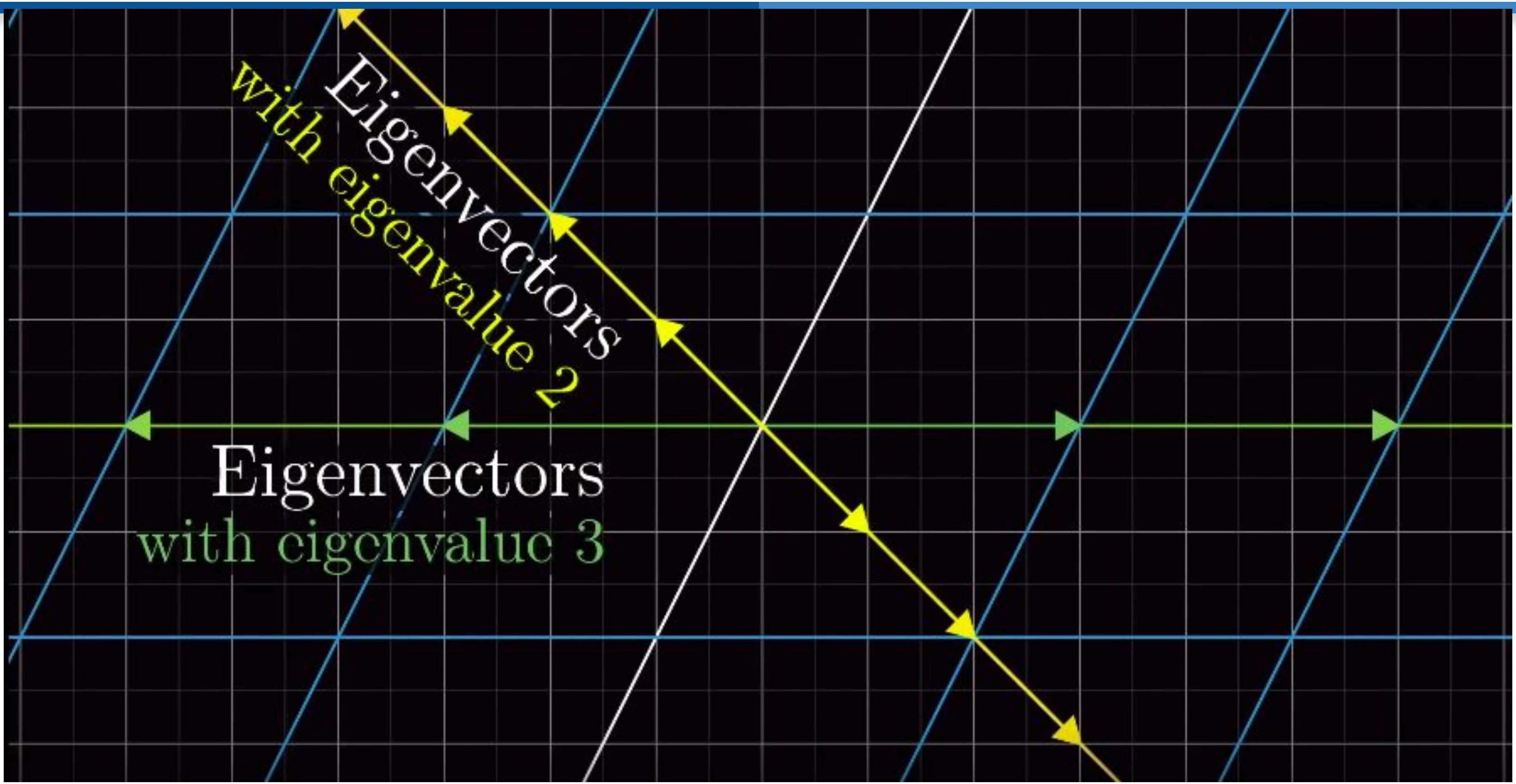

Autodecomposição

Sendo $\boldsymbol{A}$ uma matriz, **v** seus autovetores e **λ** seu autovalor, tem-se que

$$\boldsymbol{A}\boldsymbol{v} = \lambda\boldsymbol{v}.$$

Autodecomposição

Suponha que a matriz $\boldsymbol{A}$ tenha n autovetores linearmente independente (por quê?) $\{\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}\}$, com seus correspondentes autovalores $\{\lambda_1, \ldots, \lambda_n\}$:

$\boldsymbol{V} = [\mathbf{v}^{(1)}, \ldots, \mathbf{v}^{(n)}]$ (um autovetor por coluna)

$\boldsymbol{\lambda} = [\lambda_1, \ldots, \lambda_n]^T$

A **autodecomposição** de A pode ser decomposta da seguinte maneira:

$$\boldsymbol{A} = \boldsymbol{V} \operatorname{diag}(\boldsymbol{\lambda}) \boldsymbol{V}^{-1}$$

Autodecomposição

- Nem todas as matrizes podem ser decompostas em autovalores e autovetores
- Contudo, todas as **matriz real simétrica** pode ser decomposta utilizando apenas valores reais.

Autodecomposição

Seja $\boldsymbol{A}$ uma matriz real simétrica, $\boldsymbol{Q}$ uma matriz ortogonal composta pelos autovetores de $\boldsymbol{A}$ e $\boldsymbol{\Lambda}$ uma matriz diagonal, sendo que $\boldsymbol{\Lambda}_{i,i}$ é o autovalor do autovetor presente na coluna $\boldsymbol{Q}_{:,i,}$ a decomposição de $\boldsymbol{A}$ pode ser expressa por:

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top$$

Autodecomposição

Classificação de uma matriz

Positivo definitivo: Todos os seus autovalores positivos.

Positivo semi definitivo: Todos os seus autovalores positivos ou nulos.

Negativo definitivo: Todos os seus autovalores são negativos.

Negativo semi definitivo: Todos os seus autovalores são negativos ou nulos.

Principal component analysis (PCA)

- Diminuir a dimensionalidade dos dados
- Representar os dados de forma menos custosa, admitindo uma representação com perdas

Principal component analysis (PCA)

- Considere *m* vetores com *n* dimensões, $\{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(m)}\}$, sendo $\mathbf{x}^{(i)} \in \mathbb{R}^n$. O objetivo do PCA é encontrar uma representação $\mathbf{c}^{(i)}$ contendo l dimensões, ou seja, $\mathbf{c}^{(i)} \in \mathbb{R}^n$, para cada vetor $\mathbf{x}^{(i)}$.

- Para tal, definimos uma função codificadora

$$f(\boldsymbol{x}) = \boldsymbol{c}$$

e função decodificadora

$$\boldsymbol{x} \approx g(f(\boldsymbol{x})).$$

Principal component analysis (PCA)

- PCA é definido pela escolha da função decodificadora. Para simplificar, escolhemos usar uma multiplicação de matrizes

$$g(\boldsymbol{c}) = \boldsymbol{D}\boldsymbol{c}$$

$$\boldsymbol{D} \in \mathbb{R}^{n \times l}$$

- Restrições:
  - $\boldsymbol{D}$ é ortogonal!!
  - As colunos de $\boldsymbol{D}$ possuem norma 1

Principal component analysis (PCA)

- Como encontrar o ponto $\mathbf{c}^*$, que é a melhor representação possível (ponto ótimo) de x?

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} ||\boldsymbol{x} - g(\boldsymbol{c})||_2^2.$$

Principal component analysis (PCA)

- Como encontrar o ponto $\mathbf{c}^*$, que é a melhor representação possível (ponto ótimo) de $\mathbf{x}$?

$$\boldsymbol{c}^* = \arg\min_{\boldsymbol{c}} ||\boldsymbol{x} - g(\boldsymbol{c})||_2^2.$$

Pela definição da norma L^2:

$$(\boldsymbol{x} - g(\boldsymbol{c}))^\top (\boldsymbol{x} - g(\boldsymbol{c}))$$

Principal component analysis (PCA)

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Pela definição da norma L^2:

$$(\boldsymbol{x} - g(\boldsymbol{c}))^\top (\boldsymbol{x} - g(\boldsymbol{c}))$$

$$= \boldsymbol{x}^\top \boldsymbol{x} - 2\boldsymbol{x}^\top g(\boldsymbol{c}) + g(\boldsymbol{c})^\top g(\boldsymbol{c})$$

Pois $\boldsymbol{x}^\top * g(\boldsymbol{c})$ é um escalar

Principal component analysis (PCA)

$$c^* = \arg\min_{c} -2x^\top g(c) + g(c)^\top g(c)$$

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Substituindo $g(\mathrm{c}) = \boldsymbol{D}\mathrm{c}$, e $(\boldsymbol{D}\mathrm{c})^\top = \mathbf{c}^\top \boldsymbol{D}^\top$

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$$c^* = \arg\min_{c} -2x^\top Dc + c^\top D^\top Dc$$

Principal component analysis (PCA)

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Substituindo $g(\mathrm{c}) = \boldsymbol{D}\mathrm{c}$, e $(\boldsymbol{D}\mathrm{c})^\top = \mathbf{c}^\top \boldsymbol{D}^\top$

$$\begin{aligned} c^* &= \arg\min_{c} -2x^\top Dc + c^\top D^\top Dc \\ &= \arg\min_{c} -2x^\top Dc + c^\top I_l c \\ &= \arg\min_{c} -2x^\top Dc + c^\top c. \end{aligned}$$

Principal component analysis (PCA)

- Deve-se minimizar

$$\arg\min_{\boldsymbol{c}} -2\boldsymbol{x}^\top \boldsymbol{D}\boldsymbol{c} + \boldsymbol{c}^\top \boldsymbol{c}$$

Principal component analysis (PCA)

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$$\nabla_{\boldsymbol{c}}(-2\boldsymbol{x}^\top \boldsymbol{D}\boldsymbol{c} + \boldsymbol{c}^\top \boldsymbol{c}) = \boldsymbol{0}$$

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$$-2\boldsymbol{D}^\top \boldsymbol{x} + 2\boldsymbol{c} = \mathbf{0}$$

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$$\boldsymbol{c} = \boldsymbol{D}^\top \boldsymbol{x}.$$

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$$-2\boldsymbol{D}^\top \boldsymbol{x} + 2\boldsymbol{c} = \boldsymbol{0}$$

$$\boldsymbol{c} = \boldsymbol{D}^\top \boldsymbol{x}.$$

$$r(\boldsymbol{x}) = g\left(f\left(\boldsymbol{x}\right)\right) = \boldsymbol{D}\boldsymbol{D}^\top \boldsymbol{x}.$$

Principal component analysis (PCA)

- Deve-se minimizar

$$\boldsymbol{D}^* = \arg\min_{\boldsymbol{D}} \sqrt{\sum_{i,j} \left(x_j^{(i)} - r(\boldsymbol{x}^{(i)})_j \right)^2} \text{ subject to } \boldsymbol{D}^\top \boldsymbol{D} = \boldsymbol{I}_l.$$

- Restrição: l =1. Tem-se $\boldsymbol{D} = \boldsymbol{d}$, um vetor de apenas 1 coluna

$$\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}} \sum_i ||\boldsymbol{x}^{(i)} - \boldsymbol{d}\boldsymbol{d}^\top \boldsymbol{x}^{(i)}||_2^2 \text{ subject to } ||\boldsymbol{d}||_2 = 1$$

Principal component analysis (PCA)

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Principal component analysis (PCA)

$$d^* = \arg\min_{d} \sum_i ||x^{(i)} - dd^\top x^{(i)}||_2^2 \text{ subject to } ||d||_2 = 1$$

Por estética, o escalar $\boldsymbol{d}^\top \boldsymbol{x}^{(i)}$ deve ir a esquerda de $\boldsymbol{d}$

Principal component analysis (PCA)

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Como a transposta de um escalar é igual ao escalar:

Principal component analysis (PCA)

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Como a transposta de um escalar é igual ao escalar:

$$\boldsymbol{d}^* = \arg\min_{\boldsymbol{d}} \sum_i ||\boldsymbol{x}^{(i)} - \boldsymbol{x}^{(i)\top} \boldsymbol{d}\boldsymbol{d}||_2^2 \text{ subject to } ||\boldsymbol{d}||_2 = 1$$

Principal component analysis (PCA)

- Sendo $\boldsymbol{X}_{i,:} = \boldsymbol{x}^{(i)\top}$ (Mudança de notação)
- Considerando que a norma de Frobenius é equivalente a norma L^2

$$\boldsymbol{d}^* = \arg\min ||\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top||_F^2 \text{ subject to } \boldsymbol{d}^\top\boldsymbol{d} = 1$$

$$\arg\min_{\boldsymbol{d}} ||\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top||_F^2$$

- Considerando o "Operador de Rastreamento":

$$||A||_F = \sqrt{\mathrm{Tr}(\boldsymbol{A}\boldsymbol{A}^\top)}$$

- Tem-se que:

$$= \arg\min_{\boldsymbol{d}} \mathrm{Tr}\left(\left(\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top\right)^\top \left(\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top\right)\right)$$

Principal component analysis (PCA)

$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}\left(\left(\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top\right)^\top \left(\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top\right)\right)$$

Principal component analysis (PCA)

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$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X} - \boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top - \boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X} + \boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top)$$

Principal component analysis (PCA)

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$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}) - \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) - \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}) + \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top)$$

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Principal component analysis (PCA)

$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}\left(\left(\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top \right)^\top \left(\boldsymbol{X} - \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top \right) \right)$$

$$= \arg\min_{\boldsymbol{d}} \operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X} - \boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top - \boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X} + \boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top)$$

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$$= \arg\min_{\boldsymbol{d}} -2\operatorname{Tr}(\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \operatorname{Tr}(\boldsymbol{d}\boldsymbol{d}^\top\boldsymbol{X}^\top\boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top)$$

Principal component analysis (PCA)

Sendo que:

$$\mathrm{Tr}(\boldsymbol{ABC}) = \mathrm{Tr}(\boldsymbol{CAB}) = \mathrm{Tr}(\boldsymbol{BCA})$$

Tem-se que

$$= \arg\min_{\boldsymbol{d}} -2\,\mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \mathrm{Tr}(\boldsymbol{d}\boldsymbol{d}^\top \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top)$$

pode ser reescrito em:

$$= \arg\min_{\boldsymbol{d}} -2\,\mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top \boldsymbol{d}\boldsymbol{d}^\top)$$

Principal component analysis (PCA)

$$\arg\min_{\boldsymbol{d}} -2\,\mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top \boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

Principal component analysis (PCA)

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Principal component analysis (PCA)

$$\begin{aligned}
&\arg\min_{\boldsymbol{d}} -2\,\mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top \boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1 \\
&= \arg\min_{\boldsymbol{d}} -2\,\mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1 \\
&= \arg\min_{\boldsymbol{d}} -\mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1 \\
&= \arg\max_{\boldsymbol{d}} \mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1
\end{aligned}$$

Principal component analysis (PCA)

$$\arg\min_{\boldsymbol{d}} -2\,\mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top \boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

$$= \arg\min_{\boldsymbol{d}} -2\,\mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) + \mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

$$= \arg\min_{\boldsymbol{d}} -\mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

$$= \arg\max_{\boldsymbol{d}} \mathrm{Tr}(\boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}\boldsymbol{d}^\top) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

$$= \arg\max_{\boldsymbol{d}} \mathrm{Tr}(\boldsymbol{d}^\top \boldsymbol{X}^\top \boldsymbol{X}\boldsymbol{d}) \text{ subject to } \boldsymbol{d}^\top \boldsymbol{d} = 1$$

Principal component analysis (PCA)

- Essa minimização pode ser resolvida utilizando autodecomposição
- Esta derivação é específica para o caso $l = 1$.