3. Computing OT for data sciences

- Reality check
- Regularizations
- Entropic regularization

What matters for practitioners?

i.i.d samples $\boldsymbol{x_1, \dots, x_n} \sim \boldsymbol{\mu}$, $\boldsymbol{y_1, \dots, y_m} \sim \boldsymbol{\nu}$,

$$\hat{\boldsymbol{\mu}}_{\boldsymbol{n}} \stackrel{\text{def}}{=} \frac{1}{n}\sum_i \delta_{\boldsymbol{x_i}}, \hat{\boldsymbol{\nu}}_{\boldsymbol{m}} \stackrel{\text{def}}{=} \frac{1}{m}\sum_j \delta_{\boldsymbol{y_j}}$$

Computational properties

Compute/approximate $\boldsymbol{W_p}(\hat{\boldsymbol{\mu}}_{\boldsymbol{n}}, \hat{\boldsymbol{\nu}}_{\boldsymbol{m}})$?

Statistical properties

$$\mathbb{E}\left[|\boldsymbol{W_p}(\boldsymbol{\mu}, \boldsymbol{\nu}) - \boldsymbol{W_p}(\hat{\boldsymbol{\mu}}_{\boldsymbol{n}}, \hat{\boldsymbol{\nu}}_{\boldsymbol{m}})|\right] \leq f(n, m)?$$

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$$\boldsymbol{O((n+m)nm \log(n+m))}$$

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Sample Complexity

$$\text{If } \Omega = \mathbb{R}^d, d > 3$$

$$\mathbb{E}\left[\left|\boldsymbol{W_p}(\boldsymbol{\mu}, \boldsymbol{\nu}) - \boldsymbol{W_p}(\hat{\boldsymbol{\mu}}_{\boldsymbol{n}}, \hat{\boldsymbol{\nu}}_{\boldsymbol{n}})\right|\right] = O(n^{-1/d})$$

- [**Dudley'69**][**Dereich+'11**][**Fournier+'13**] *& others..*
- [**Weed+'17**]: sharper results when measures' support has "low effective *d*" in metric spaces
- [**Weed+'19**] for smooth densities
- **Lower bounds:** optimal quantization error.

From theory to practice ?

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Statistical properties

$$\mathbb{E}\left[|W_p(\mu,\nu) - W_p(\hat{\mu}_n,\hat{\nu}_n)|\right] = O(n^{-1/d})$$

If we use OT in data sciences we <u>must</u> regularize the problem to improve on both aspects!

Many ways to regularize (dual) OT

$$\sup_{\boldsymbol{\varphi}(x)+\boldsymbol{\psi}(y)\leq \boldsymbol{c}(x,y)} \int \boldsymbol{\varphi} d\boldsymbol{\mu} + \int \boldsymbol{\psi} d\boldsymbol{\nu}.$$

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- RKHS for potentials **[GCBP'16]**, dualize/smooth indicator constraint

$$W_1(\mu,\nu) = \sup_{\varphi \text{ 1-Lipschitz}} \int \varphi(d\mu - d\nu).$$

- Parameterize functions using ReLU Deep net with bounded weights **[ACB'17]** or use Wavelet decompositions **[Shirdhonkar+'08]** for low *d*.

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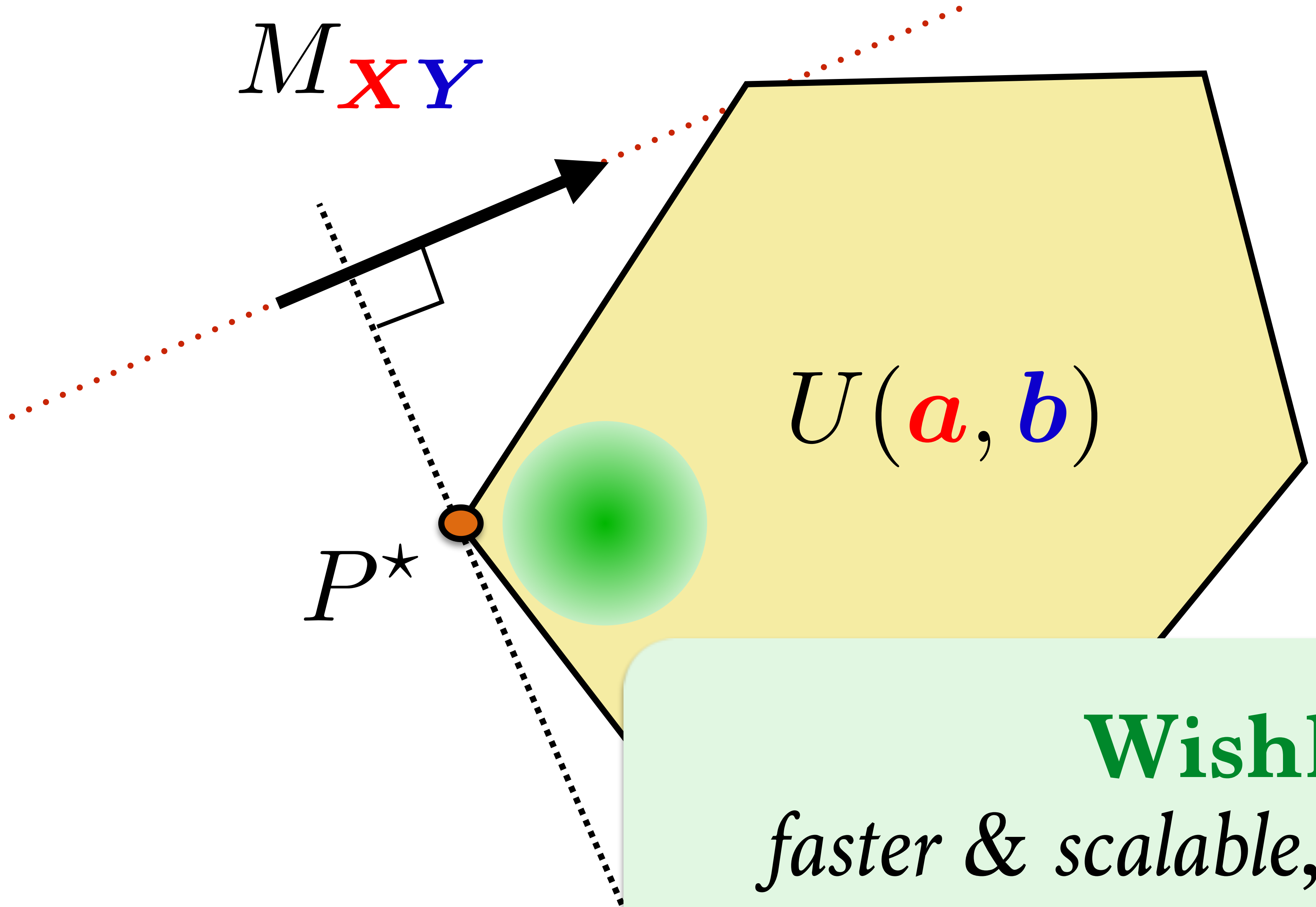
- Add prior on coupling, e.g. (entropic) regularization [C'13][GP'16][GCBCP'19][JMPC'20]

Regularization on the Primal



Wishlist:
faster & *scalable*, more *stable*,
(automatically) differentiable

Entropic Regularization [Wilson'69]

Def. Regularized Wasserstein, $\gamma \geq 0$

$$W_\gamma(\boldsymbol{\mu}, \boldsymbol{\nu}) \stackrel{\text{def}}{=} \min_{\boldsymbol{P} \in U(\boldsymbol{a}, \boldsymbol{b})} \langle \boldsymbol{P}, M_{\boldsymbol{X}\boldsymbol{Y}} \rangle - \gamma E(\boldsymbol{P})$$

$$E(P) \stackrel{\text{def}}{=} - \sum_{i,j=1}^{nm} P_{ij}(\log P_{ij} - 1)$$

Note: Unique optimal solution because of strong concavity of entropy

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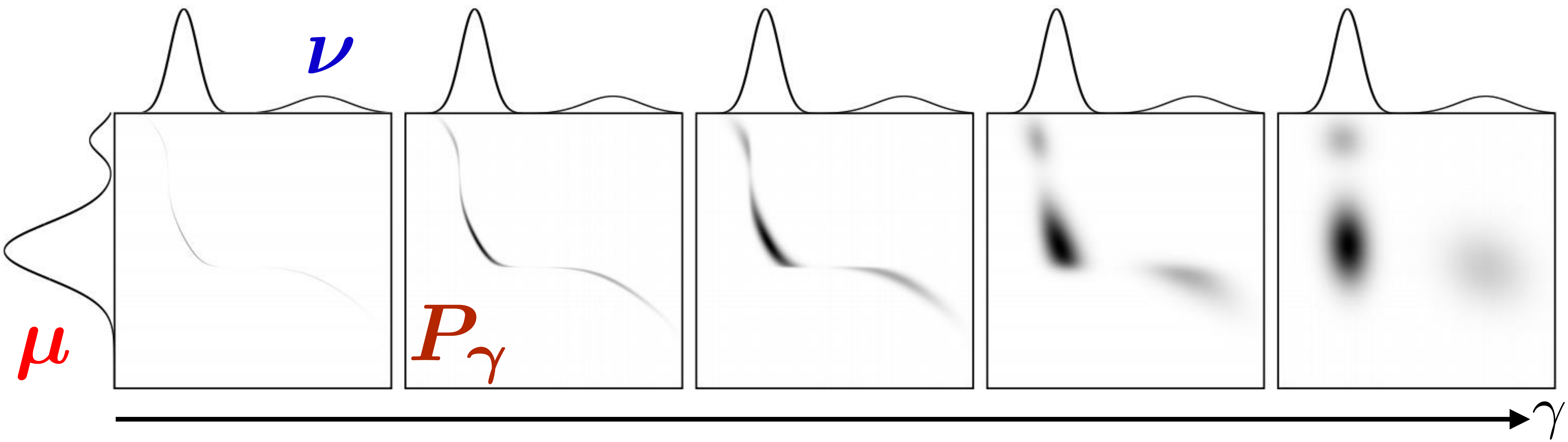

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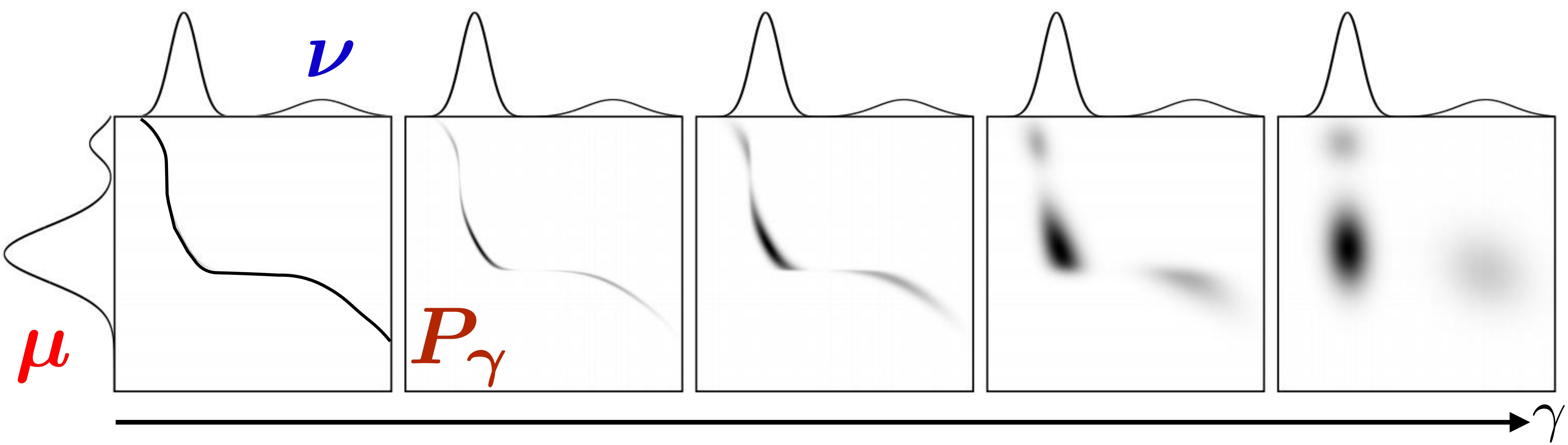

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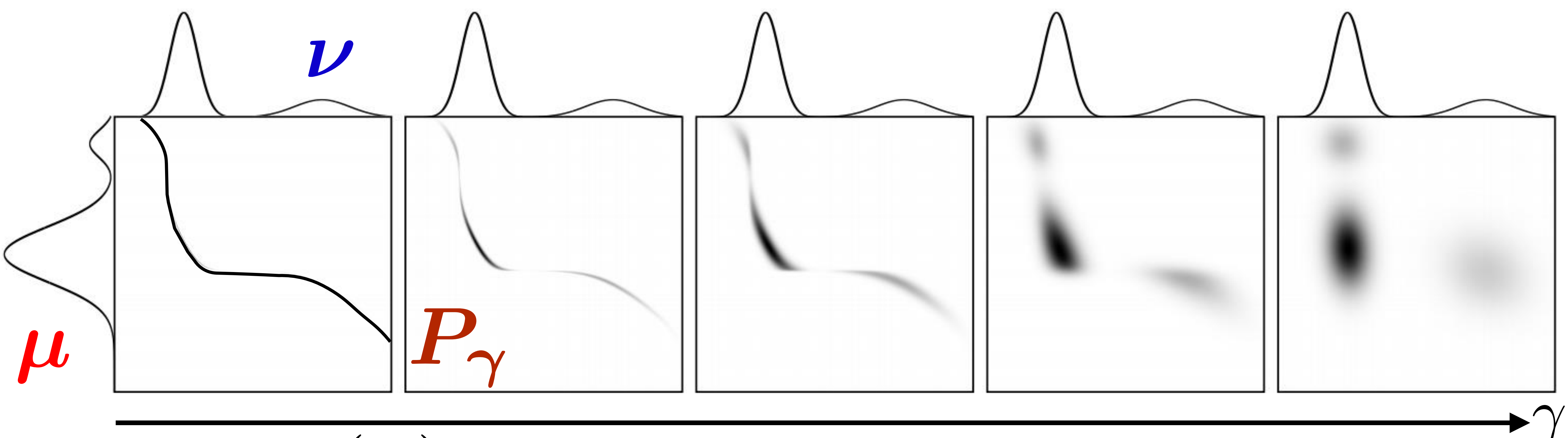

$\approx$ "$\boldsymbol{y} = \boldsymbol{T}(\boldsymbol{x})$"

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Fast & Scalable Algorithm

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then $\exists! \boldsymbol{u} \in \mathbb{R}_+^n, \boldsymbol{v} \in \mathbb{R}_+^m$, such that

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$$L(P,\alpha,\beta) = \boxed{\sum_{ij} P_{ij} M_{ij} + \gamma P_{ij}(\log P_{ij} - 1)} + \boxed{\alpha^T(P\mathbf{1} - \boldsymbol{a}) + \beta^T(P^T\mathbf{1} - \boldsymbol{b})}$$

$$\partial L/\partial P_{ij} = M_{ij} + \gamma \log P_{ij} + \alpha_i + \beta_j$$

$$(\boldsymbol{\partial L/\partial P_{ij}} = 0) \Rightarrow P_{ij} = \boldsymbol{e}^{\frac{\boldsymbol{\alpha_i}}{\gamma}} e^{-\frac{M_{ij}}{\gamma}} \boldsymbol{e}^{\frac{\boldsymbol{\beta_j}}{\gamma}} = \boldsymbol{u_i} K_{ij} \boldsymbol{v_j}$$

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Sinkhorn's Algorithm : Repeat

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- [**Sinkhorn'64**] proved first convergence result [**Franklin+'89**] characterised linear convergence
- Recent wave of great results by [**Altschuler+'17**] [**Dvurechensky+18**][**Lin+19**]
- $O(nm)$ complexity, GPGPU parallel [**C'13**] .
- $O(n \log n)$ on gridded spaces using convolutions. [**Solomon'+15**]

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- **[Sinkhorn'64]** fixed-point iterations for $(\boldsymbol{u}, \boldsymbol{v})$

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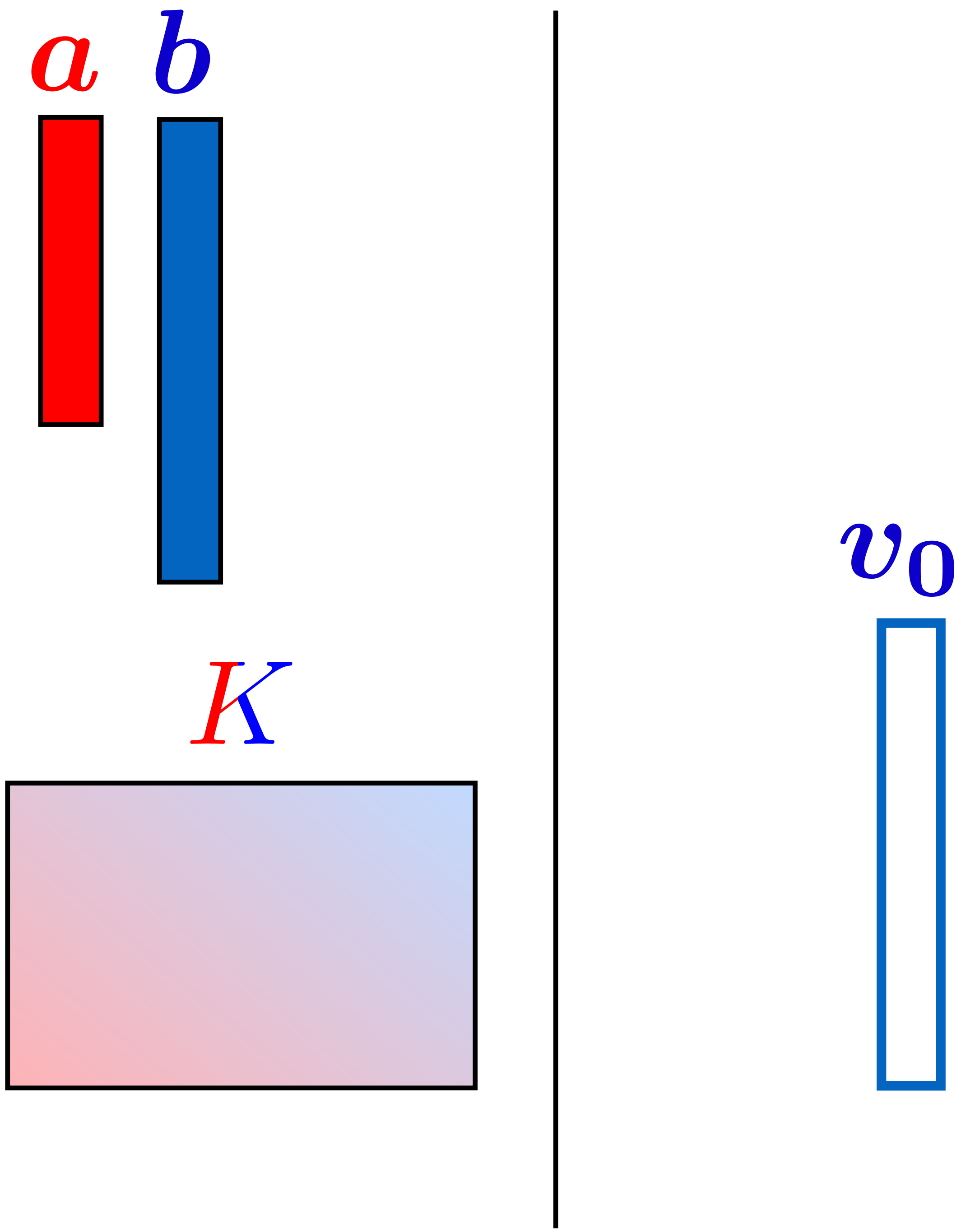

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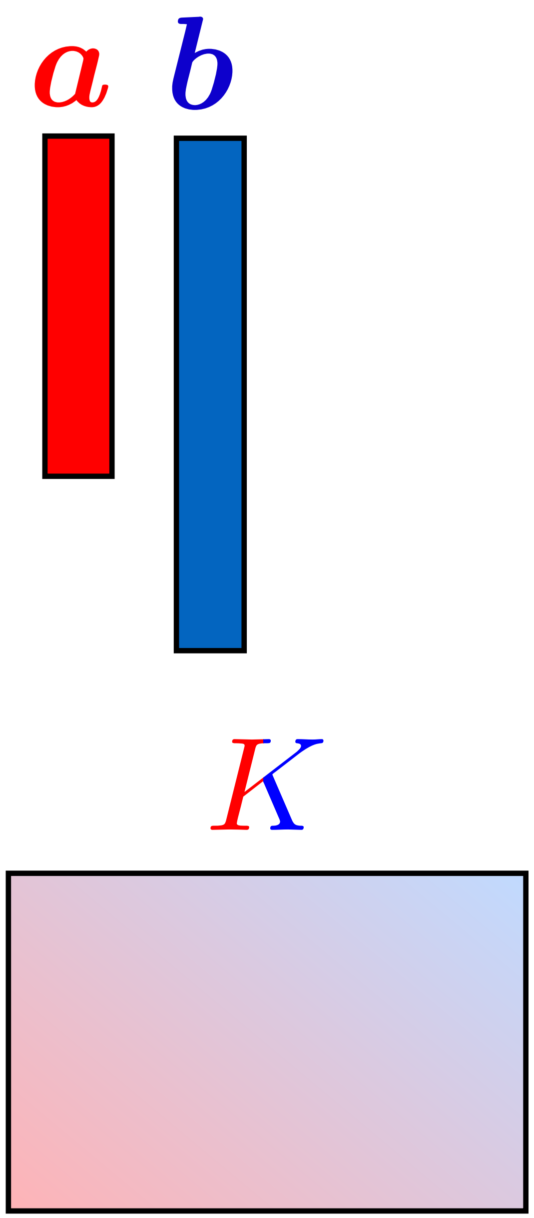

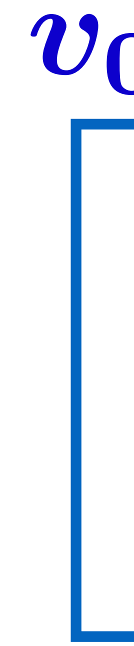

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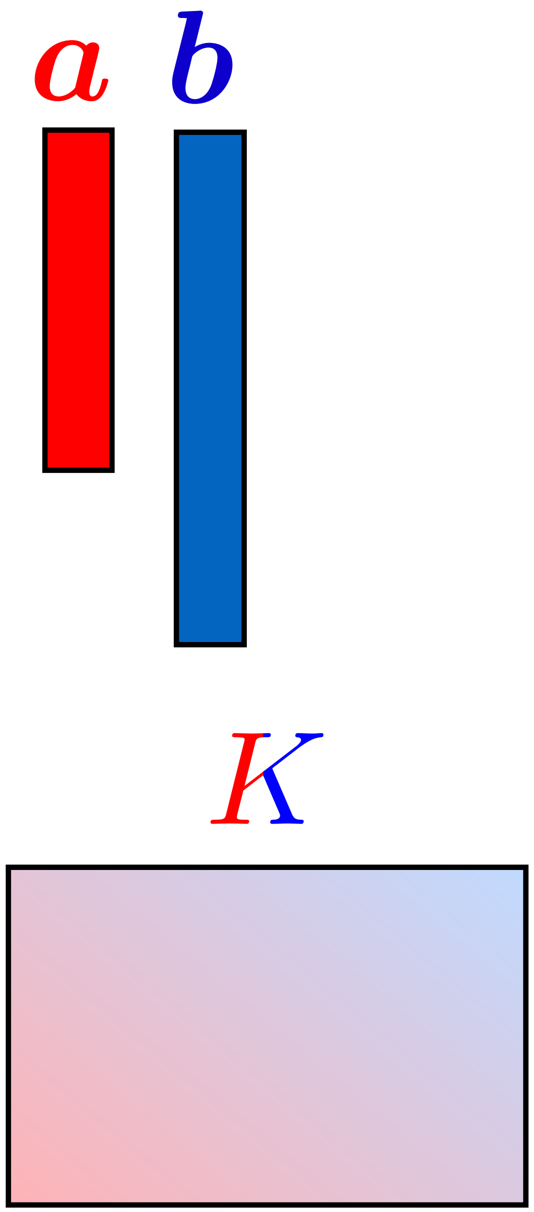

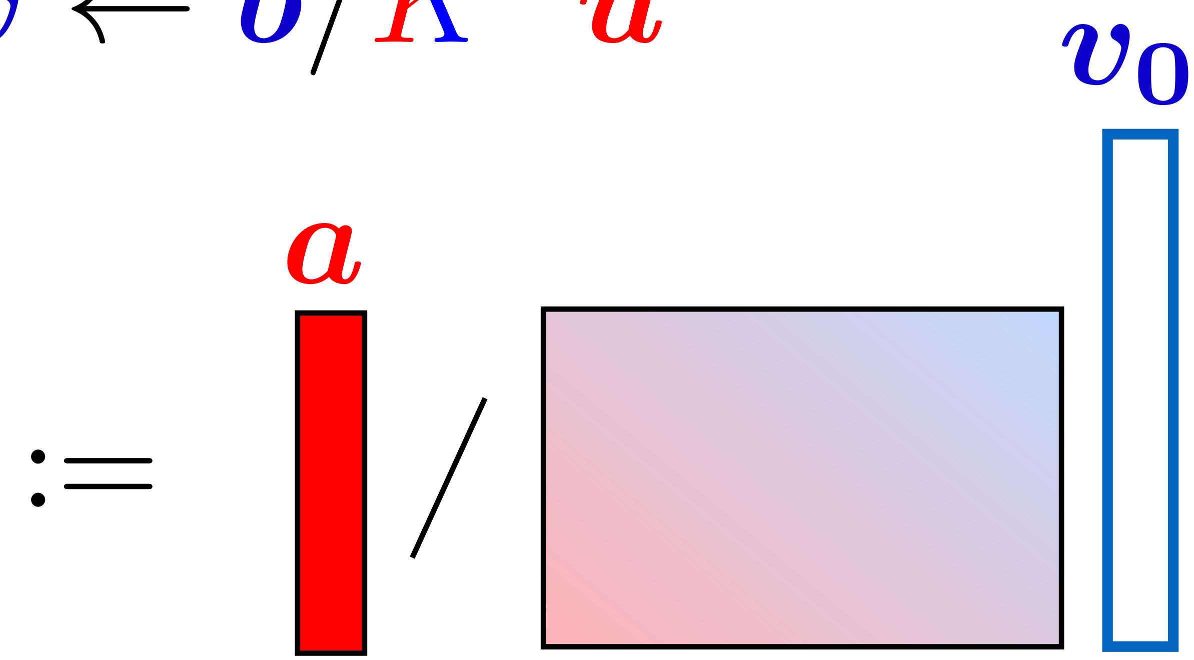

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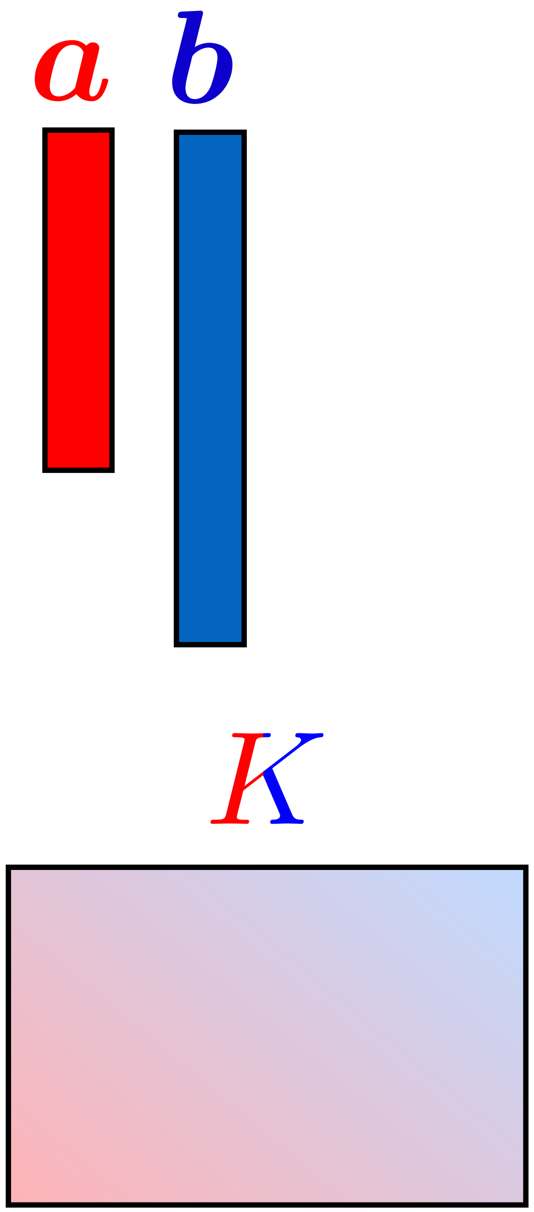

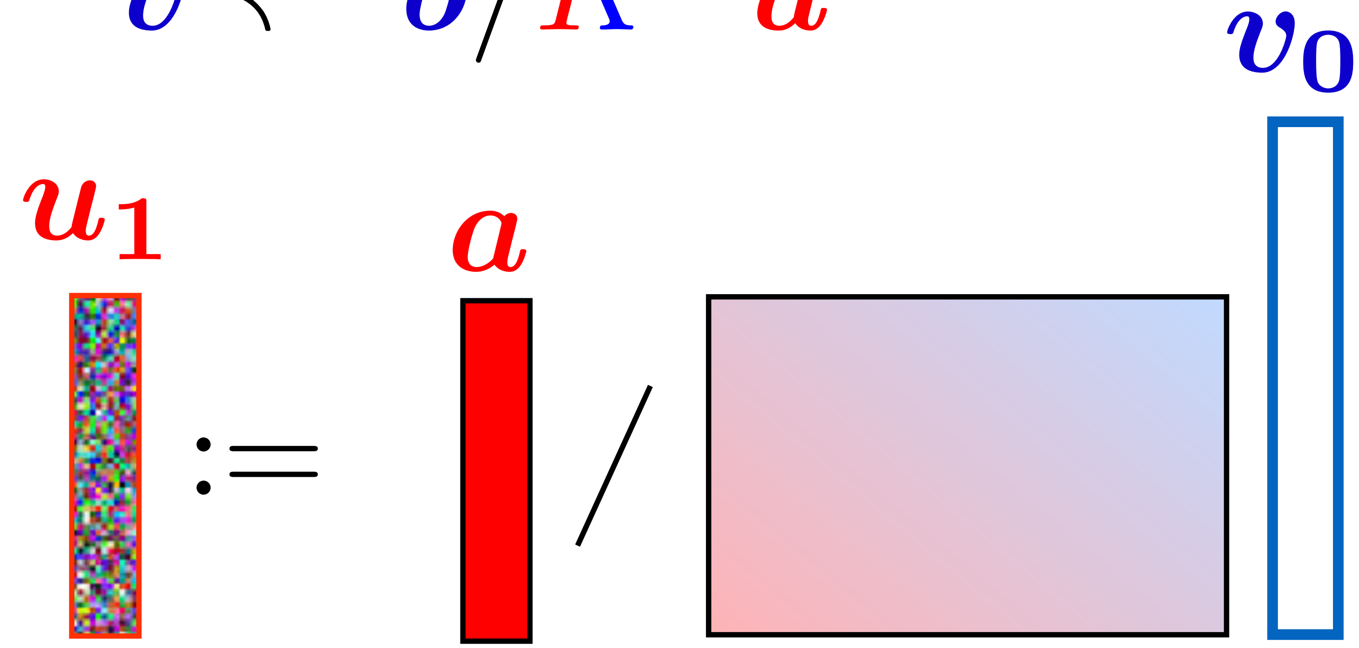

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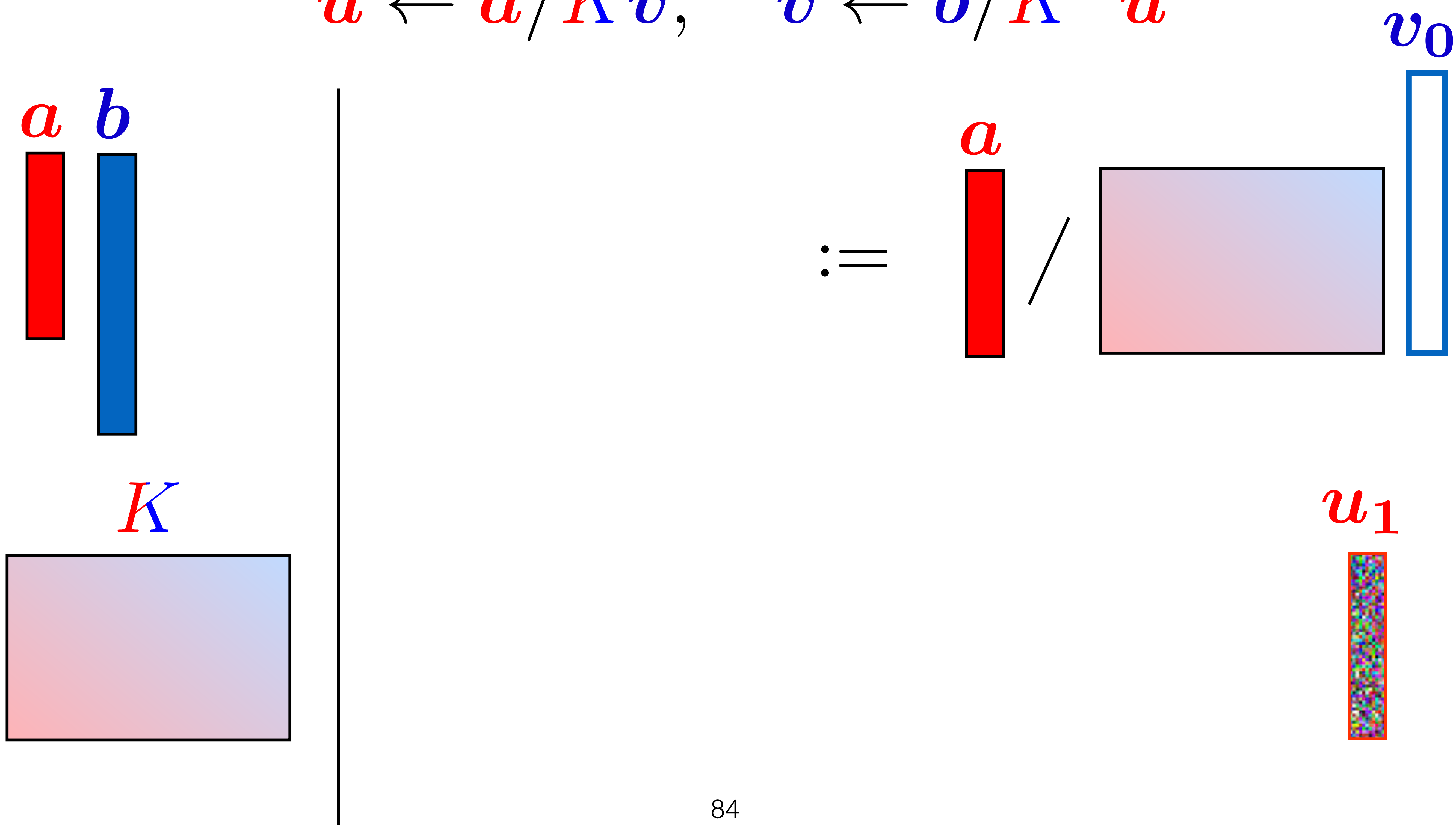

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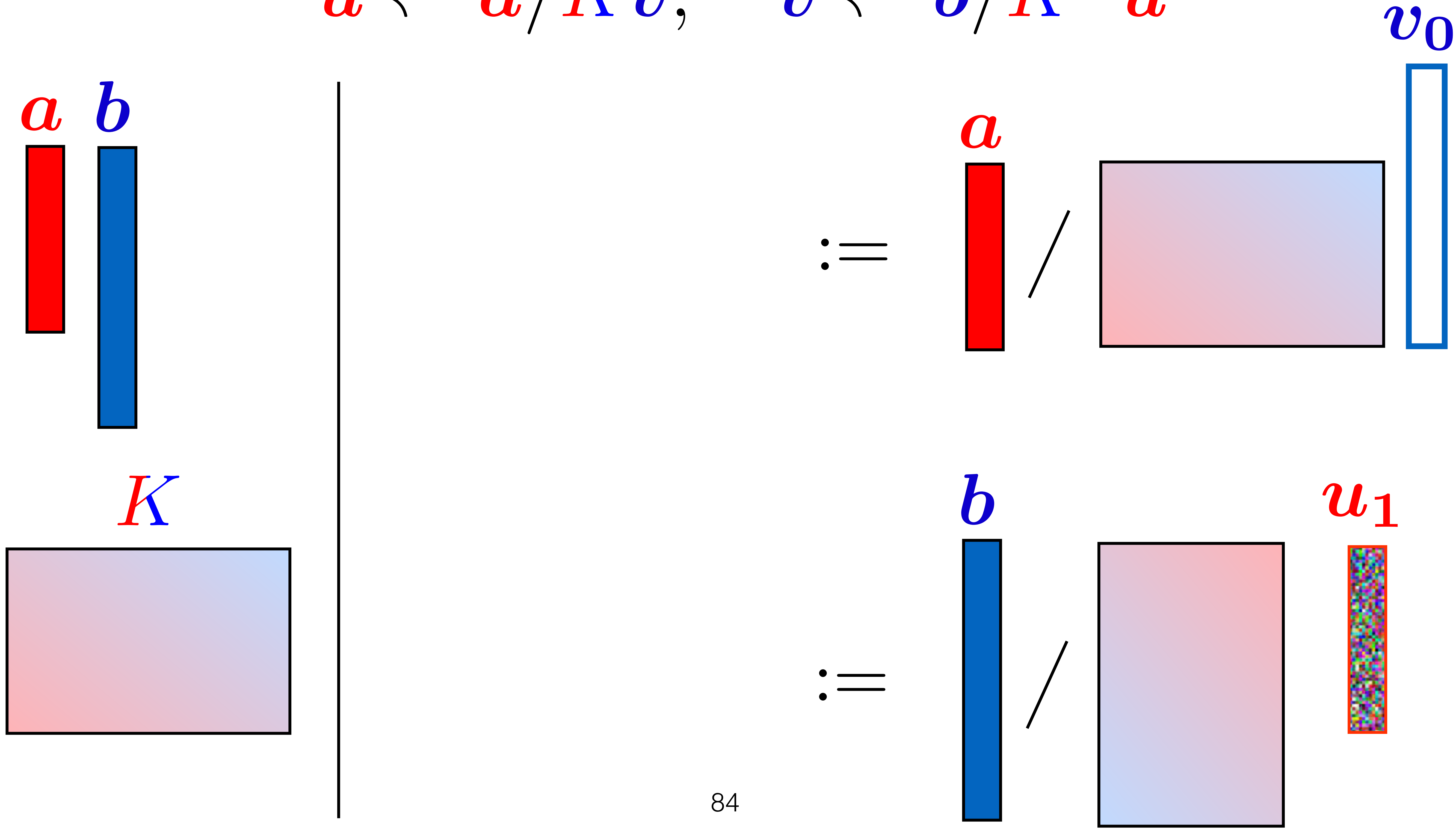

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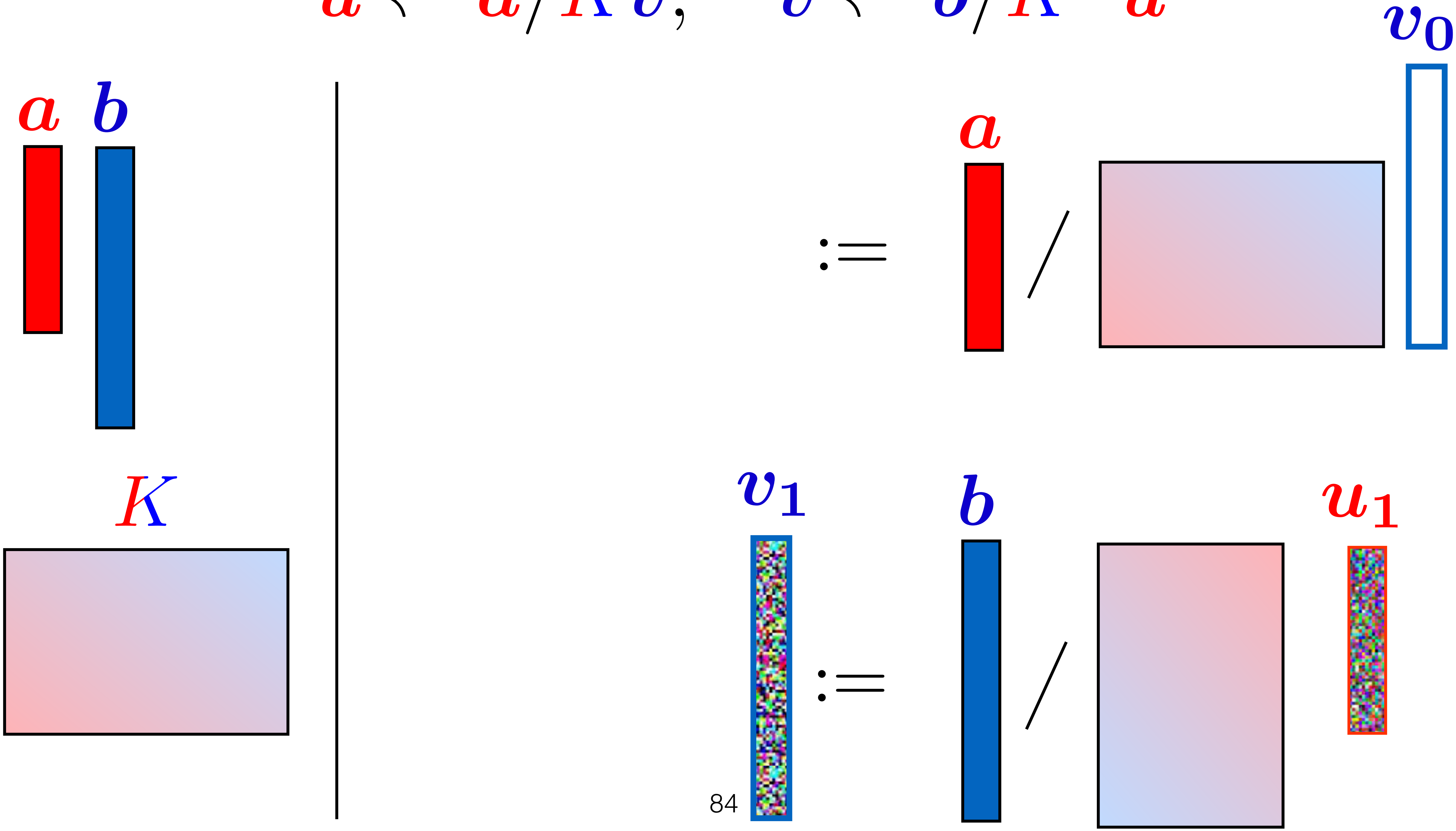

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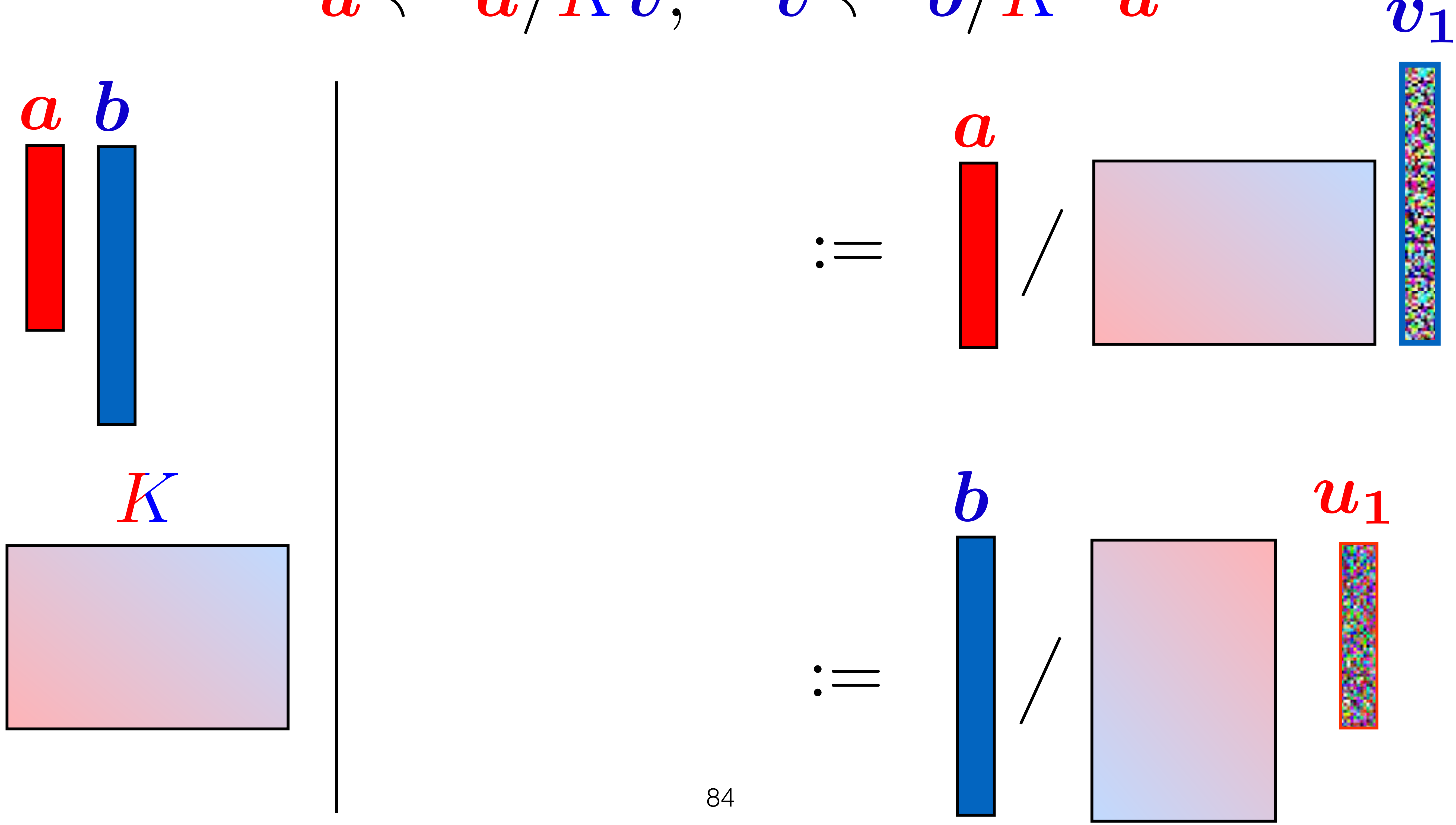

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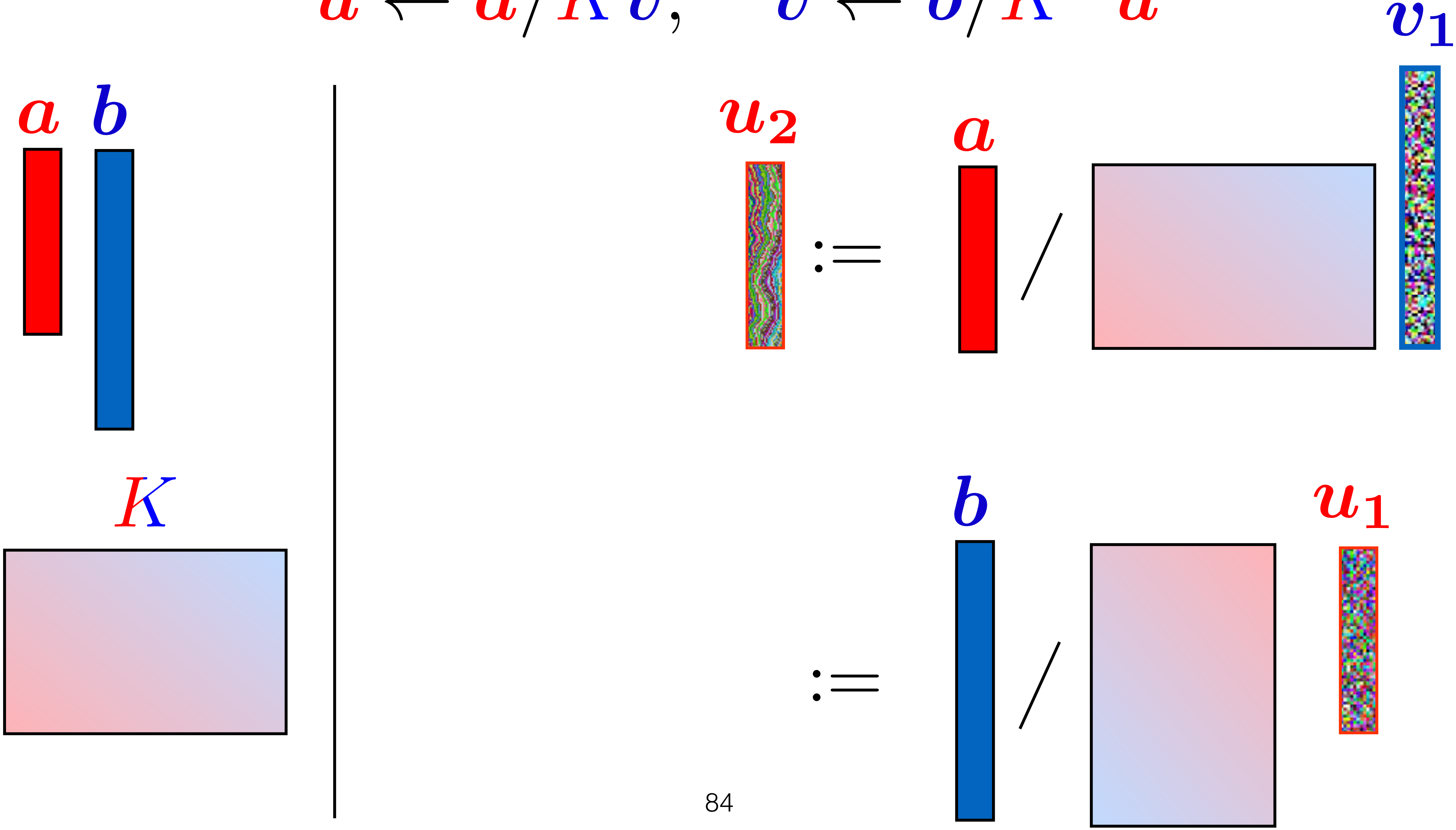

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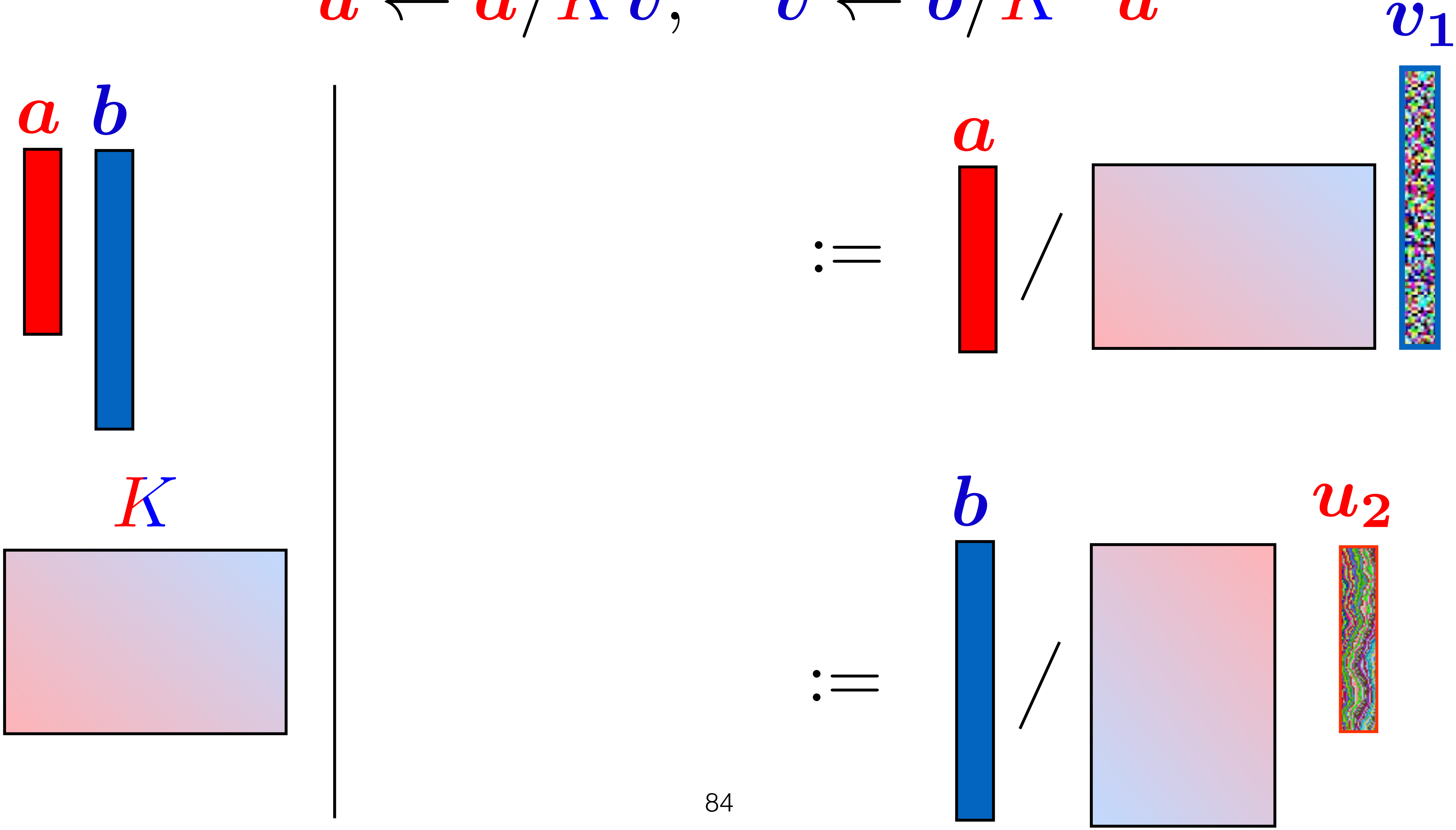

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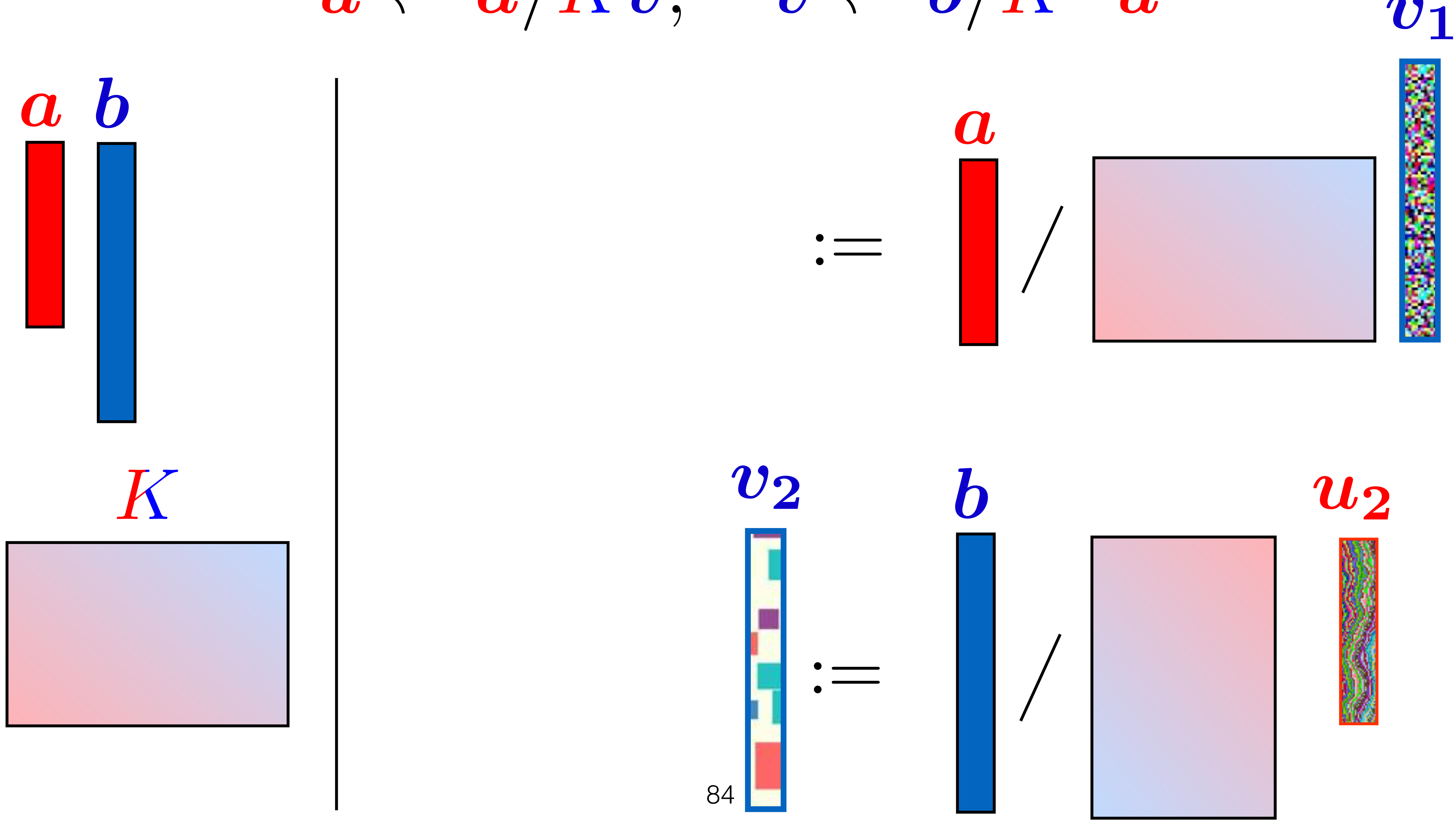

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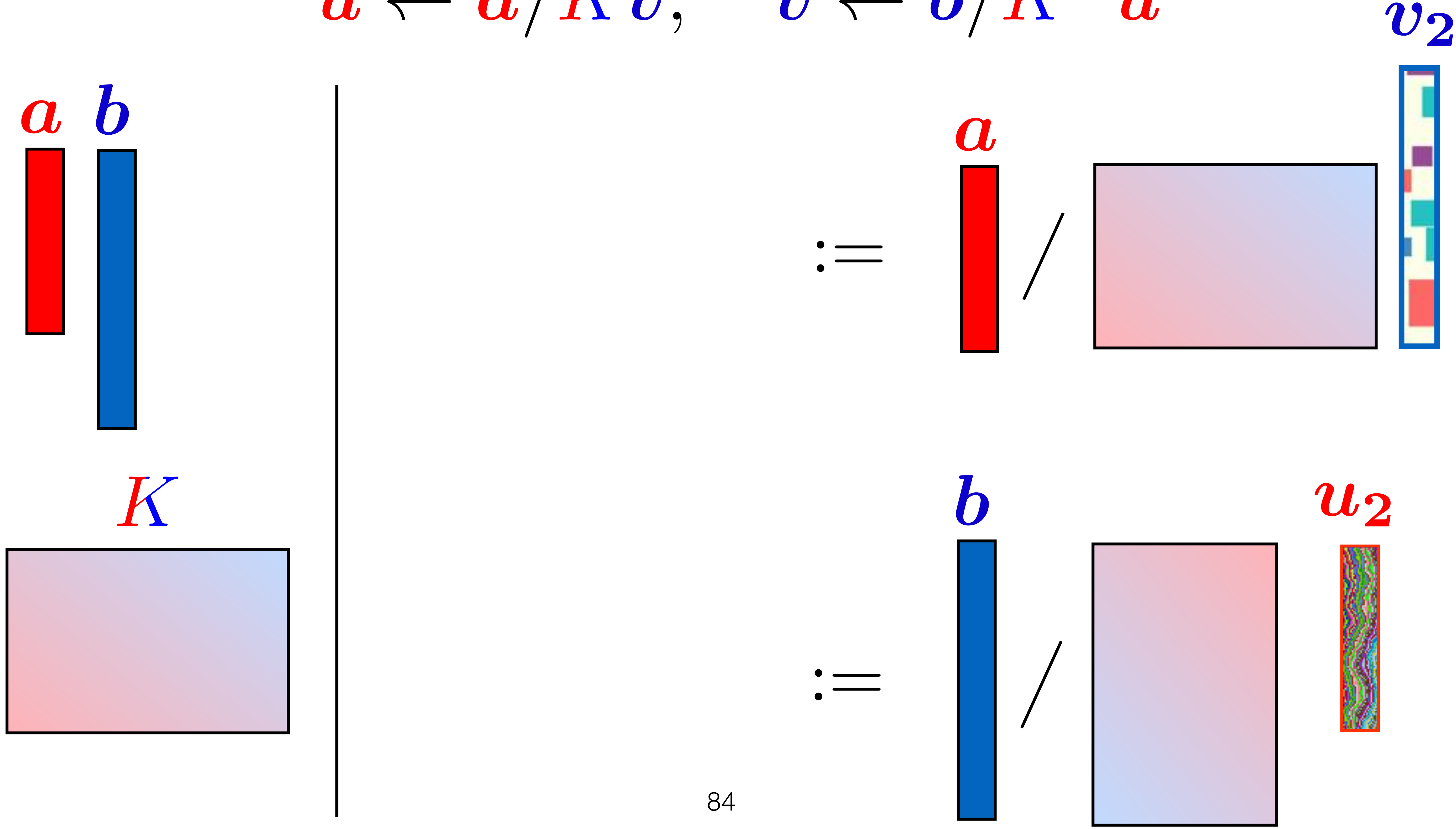

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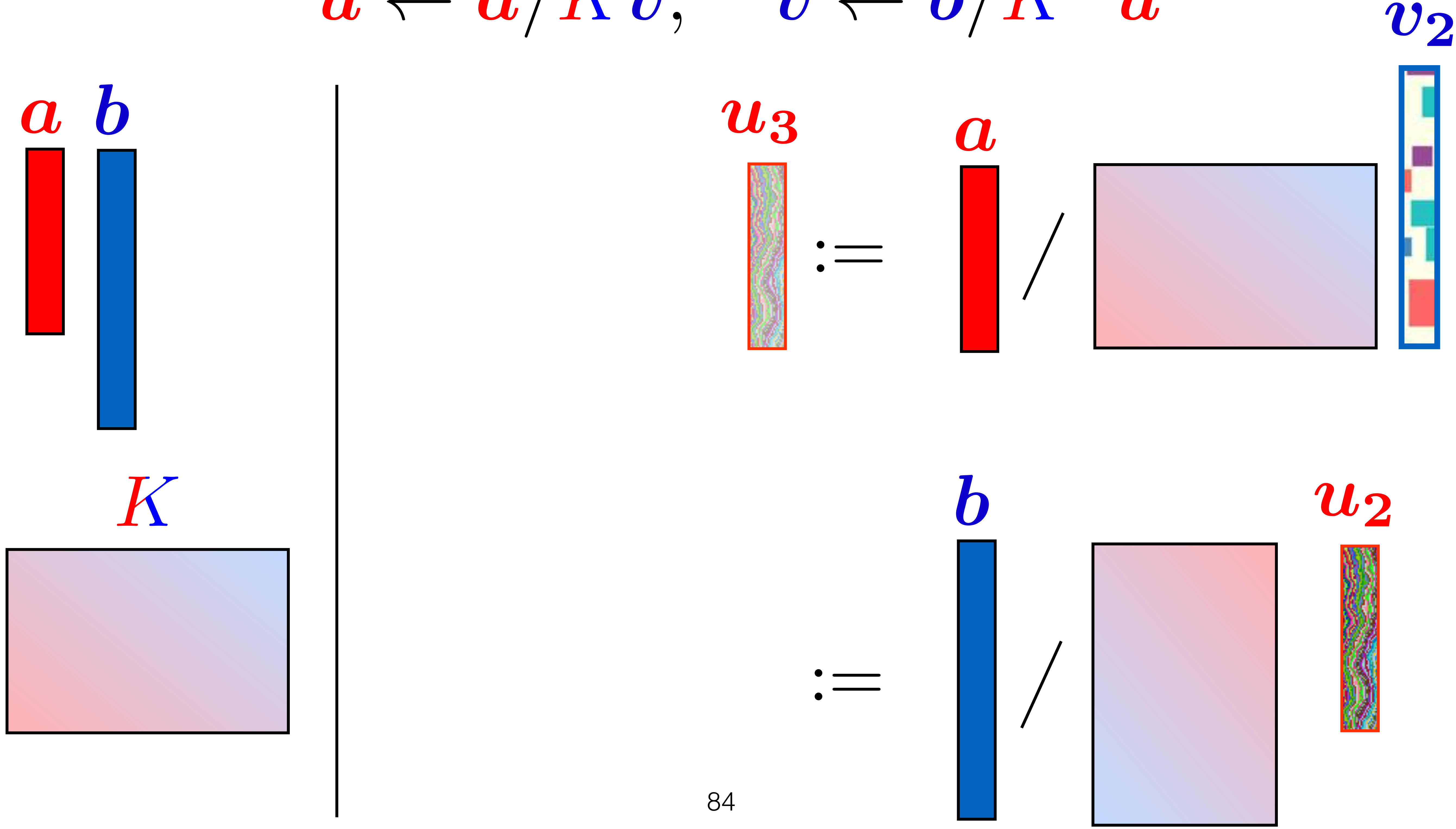

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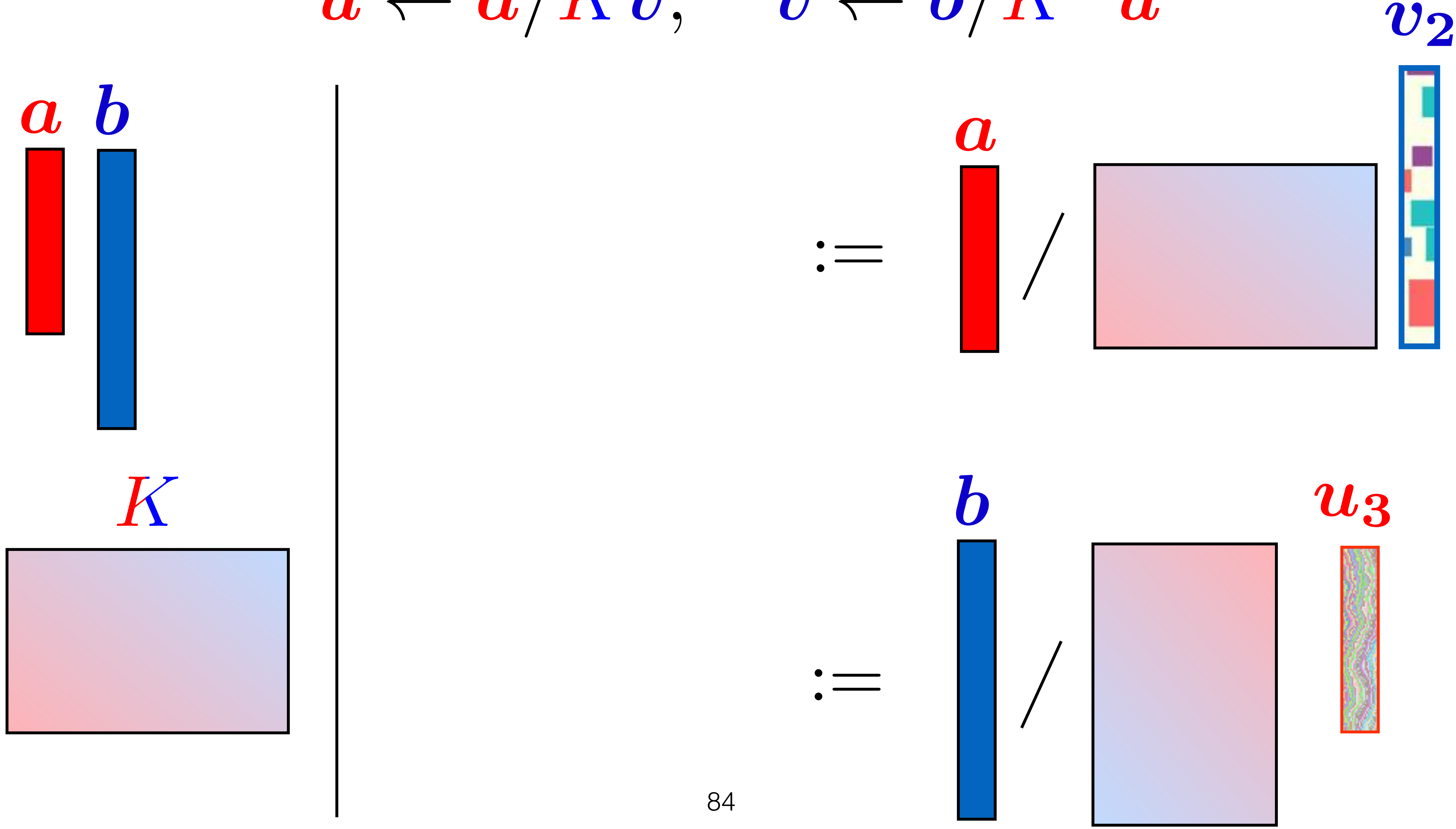

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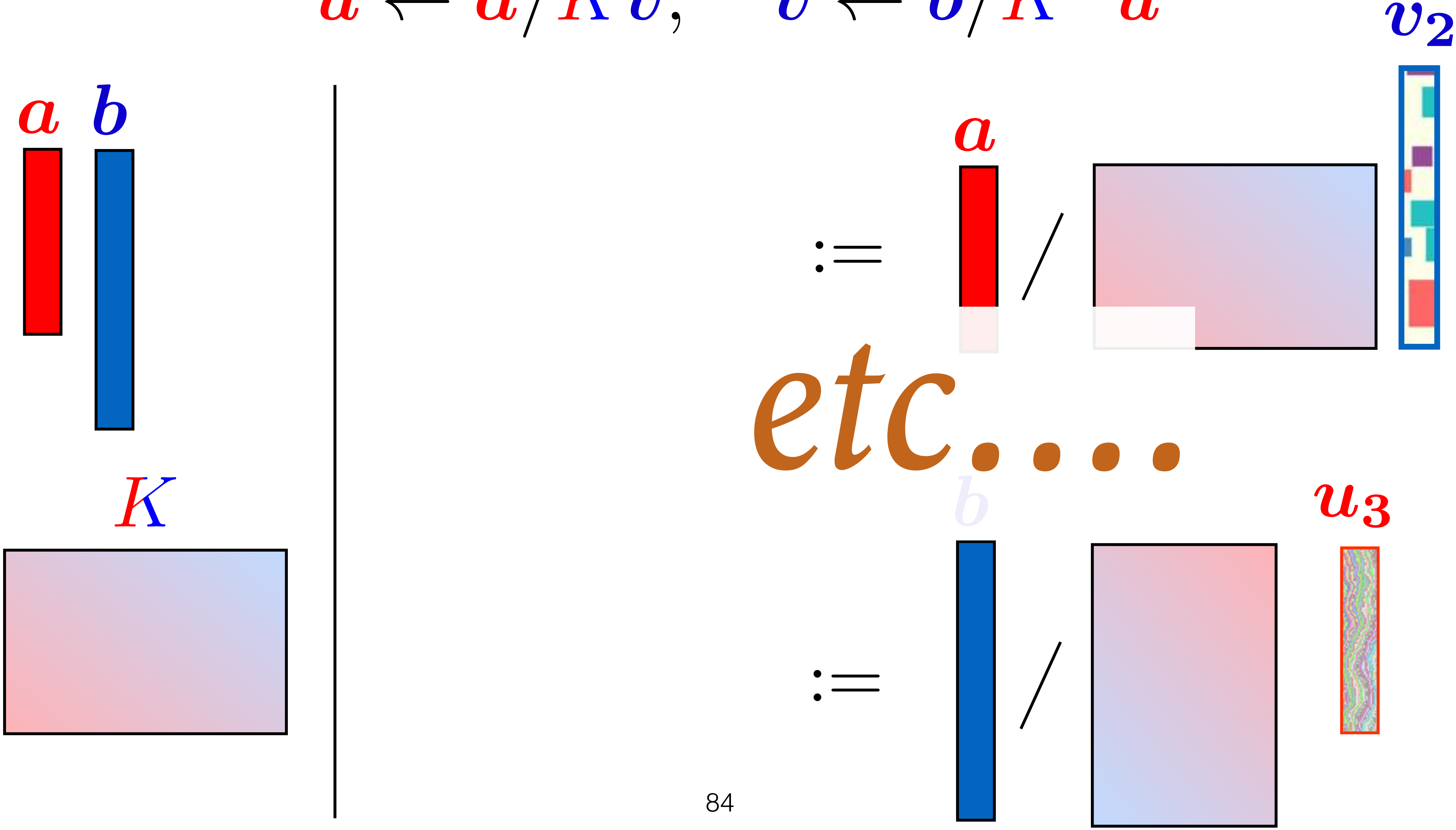
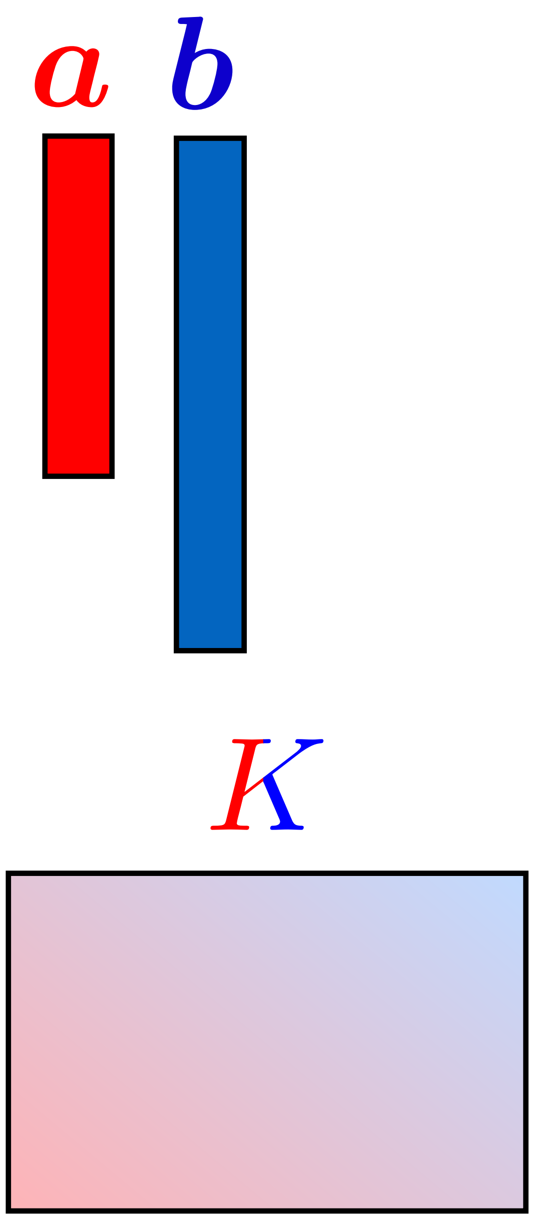
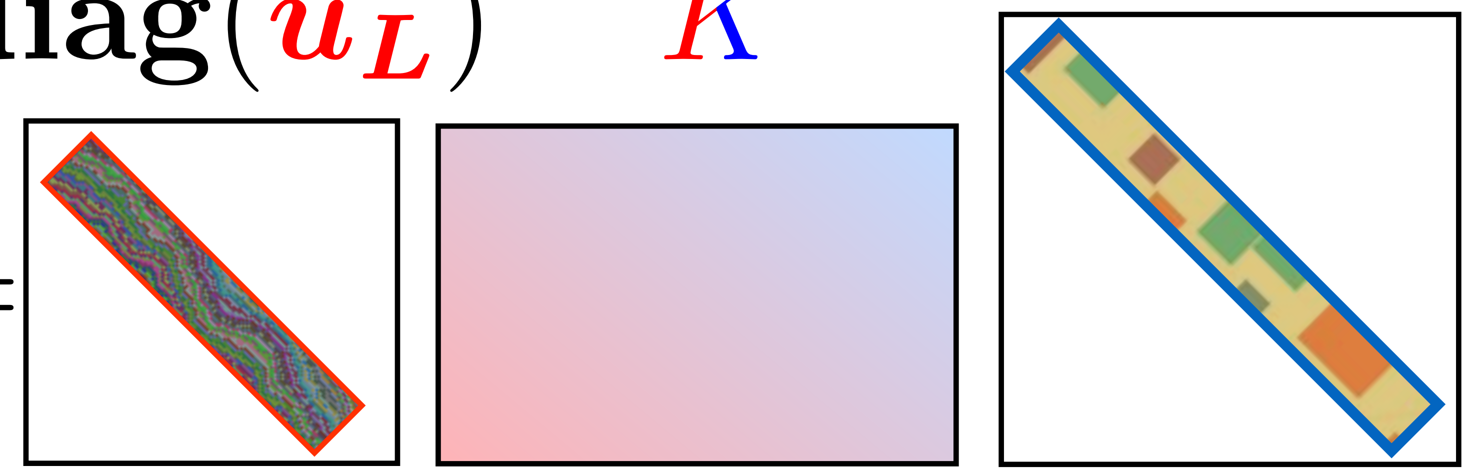


Fast & Scalable Algorithm

- **[Sinkhorn'64]** fixed-point iterations.



$$P_L := \mathbf{diag}(u_L)\, K\, \mathbf{diag}(v_L)$$



Fast & Scalable Algorithm

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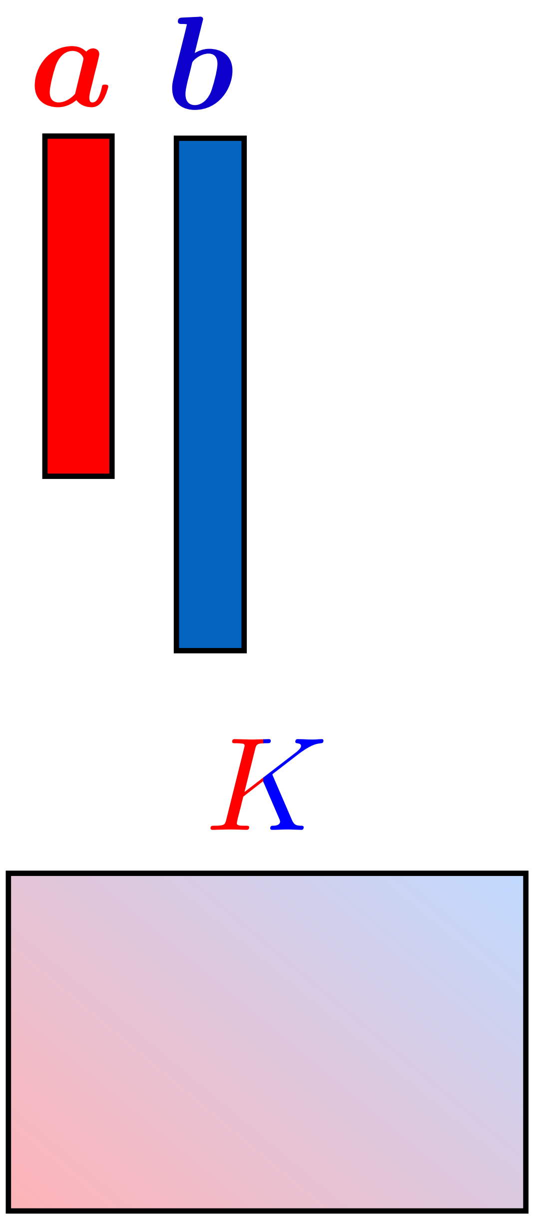
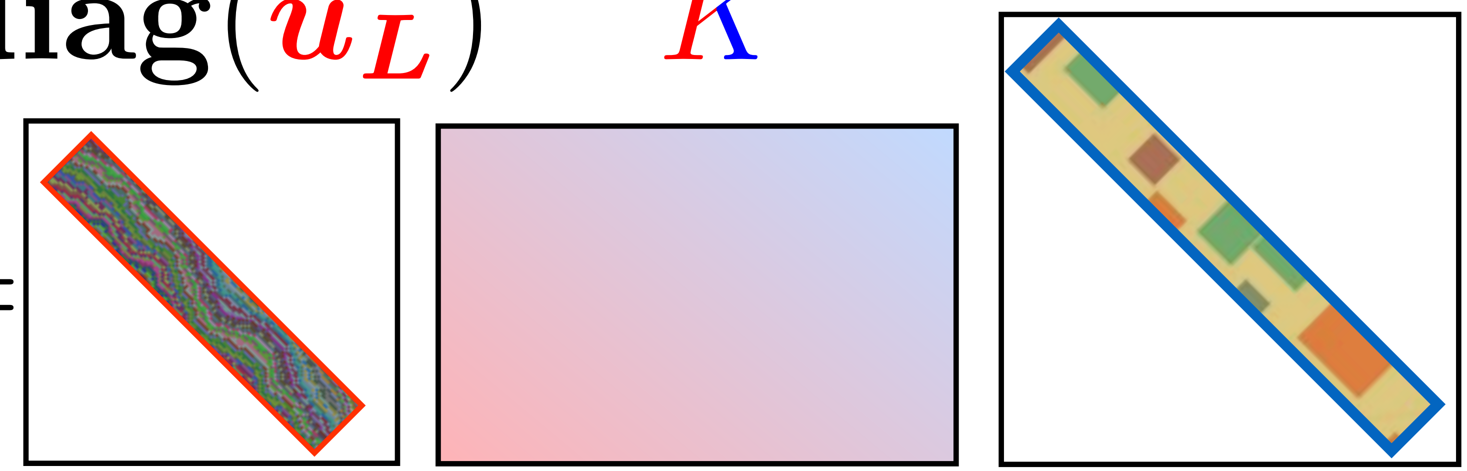
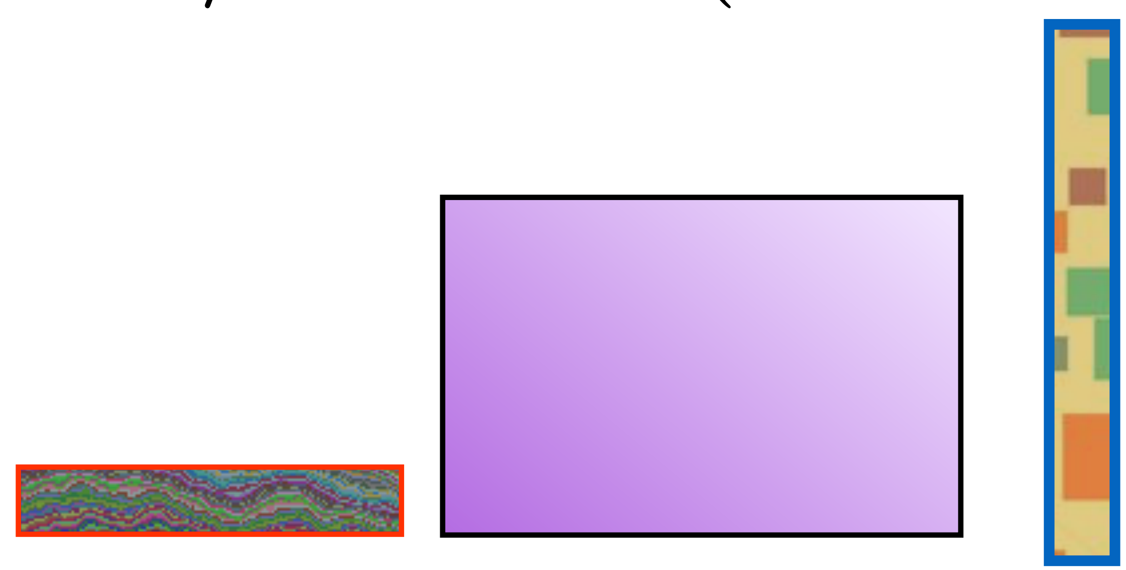


$$P_L := \mathbf{diag}(\boldsymbol{u_L})\, K\, \mathbf{diag}(\boldsymbol{v_L})$$

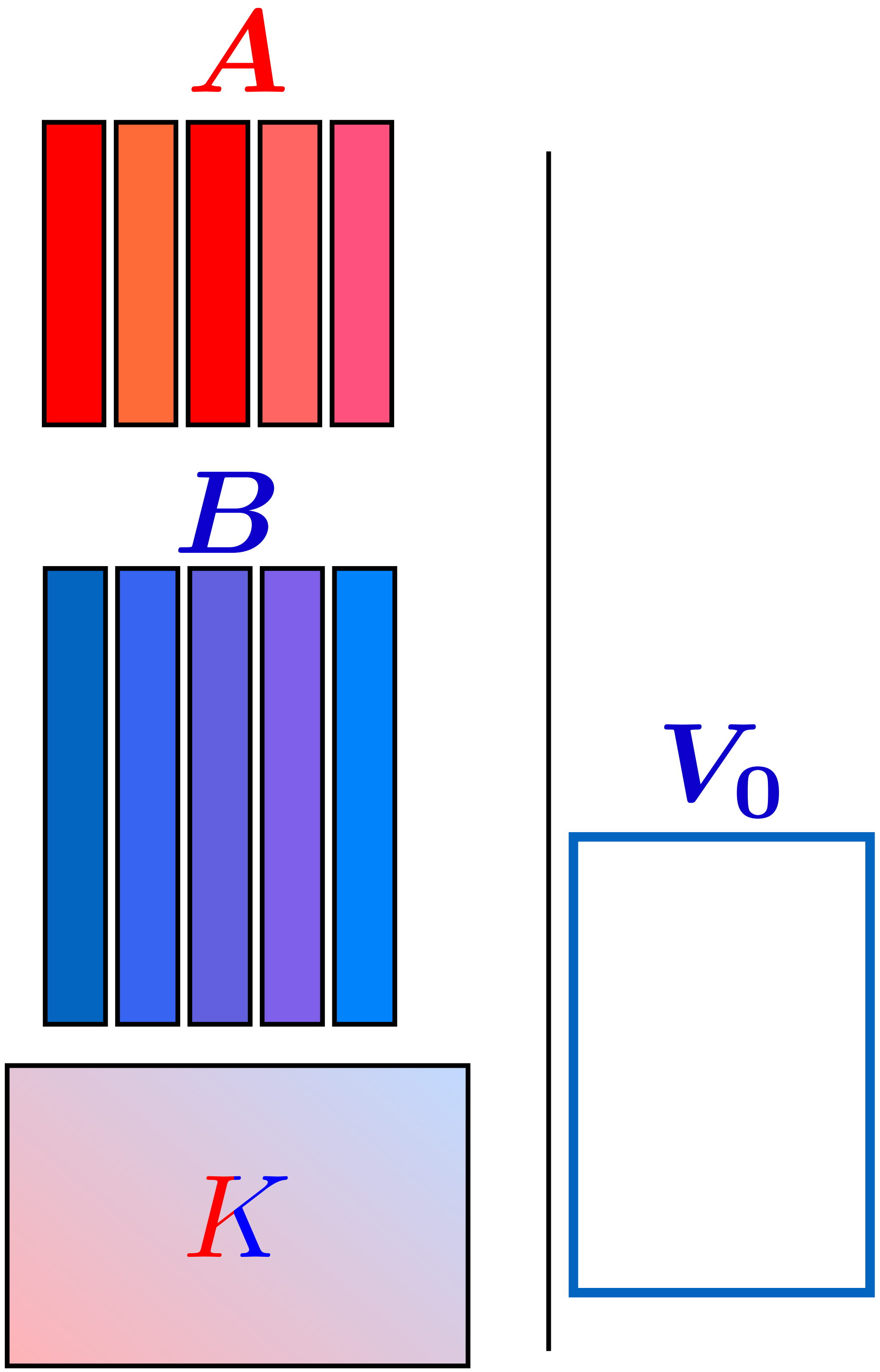


$$\langle P_L, M_{\boldsymbol{XY}} \rangle = \boldsymbol{u_L}^T (K \odot M_{\boldsymbol{XY}}) \boldsymbol{v_L}$$



Also embarrassingly parallel

- **[Sinkhorn'64]** with *matrix* fixed-point iterations



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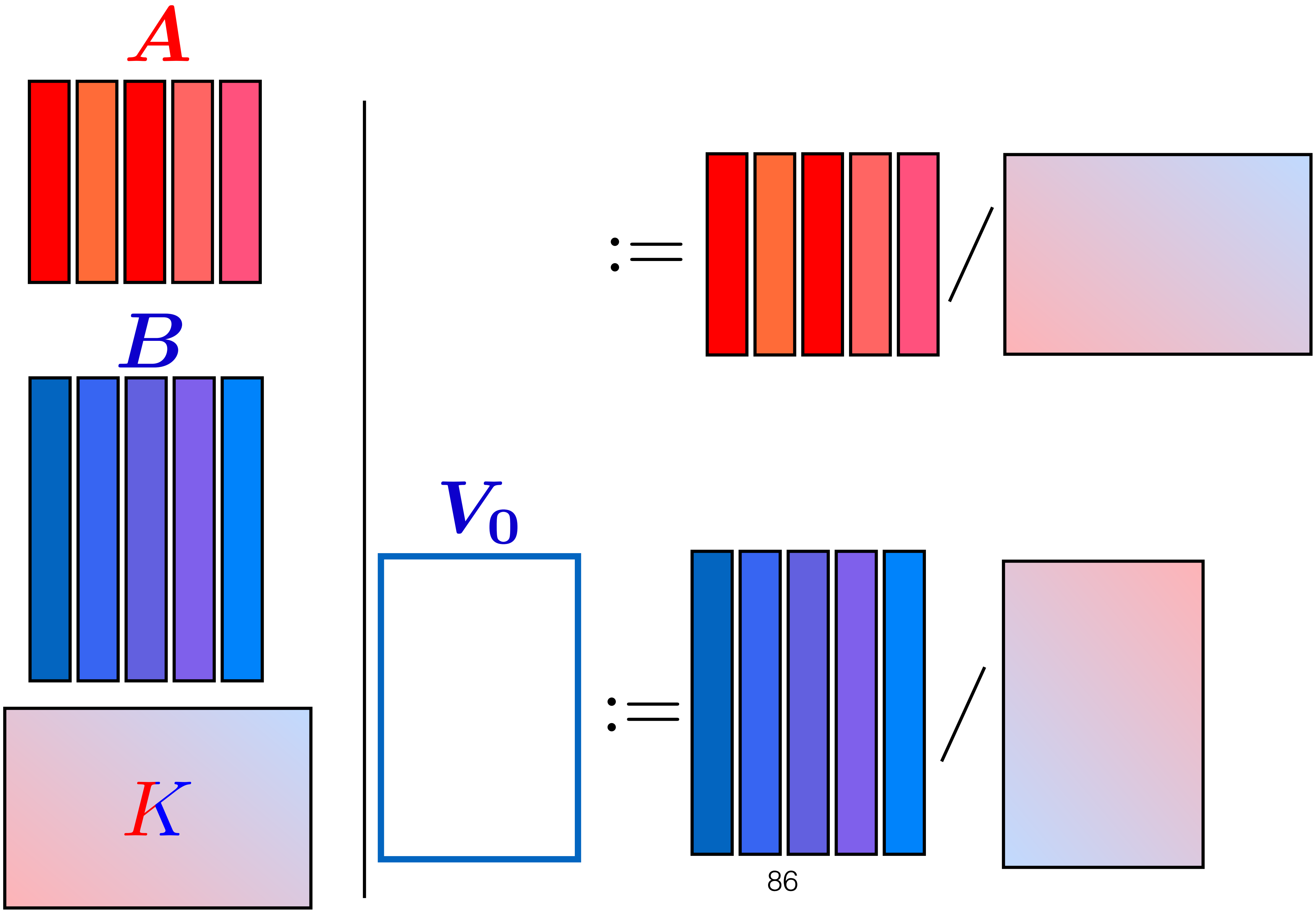

Also embarrassingly parallel

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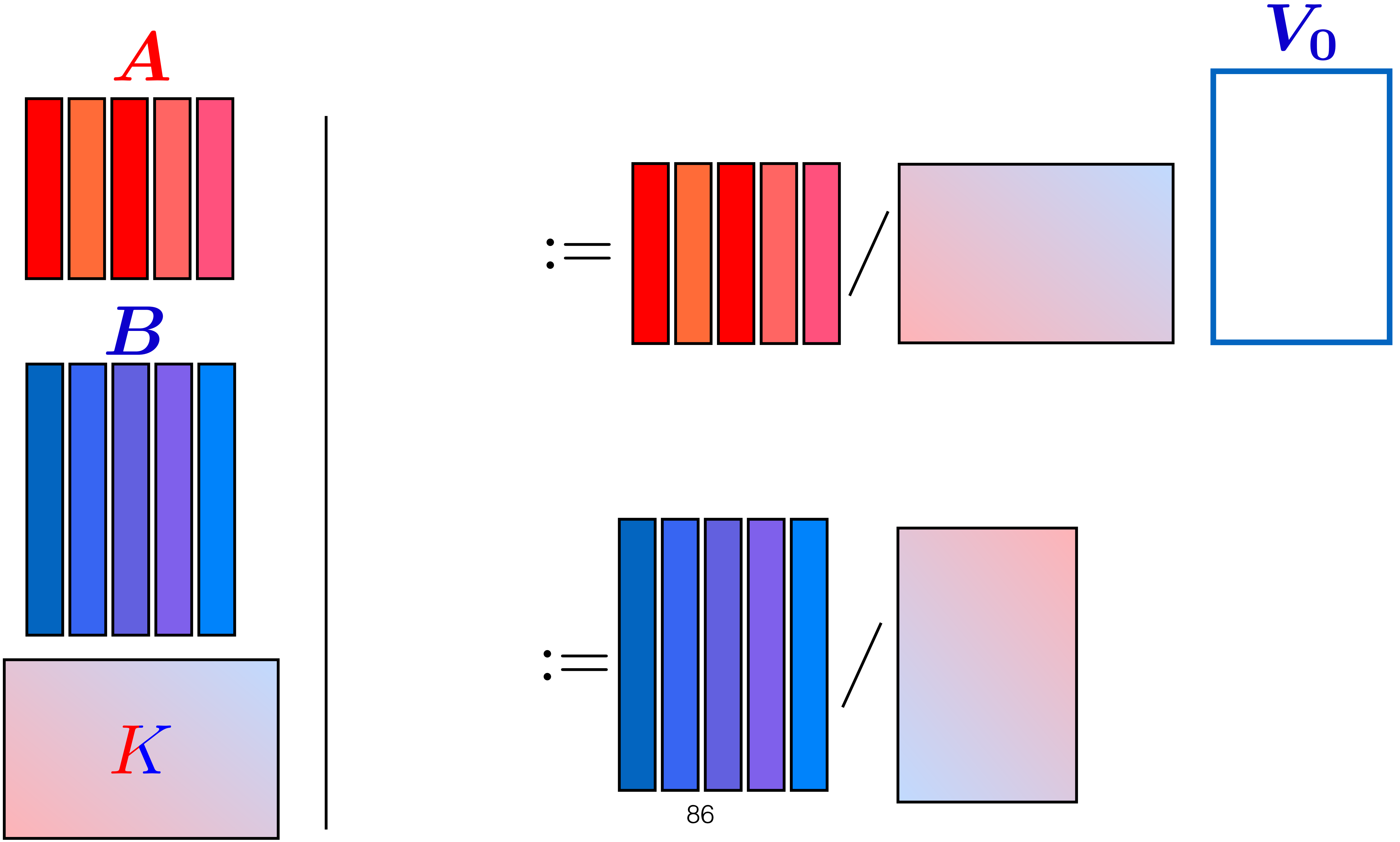

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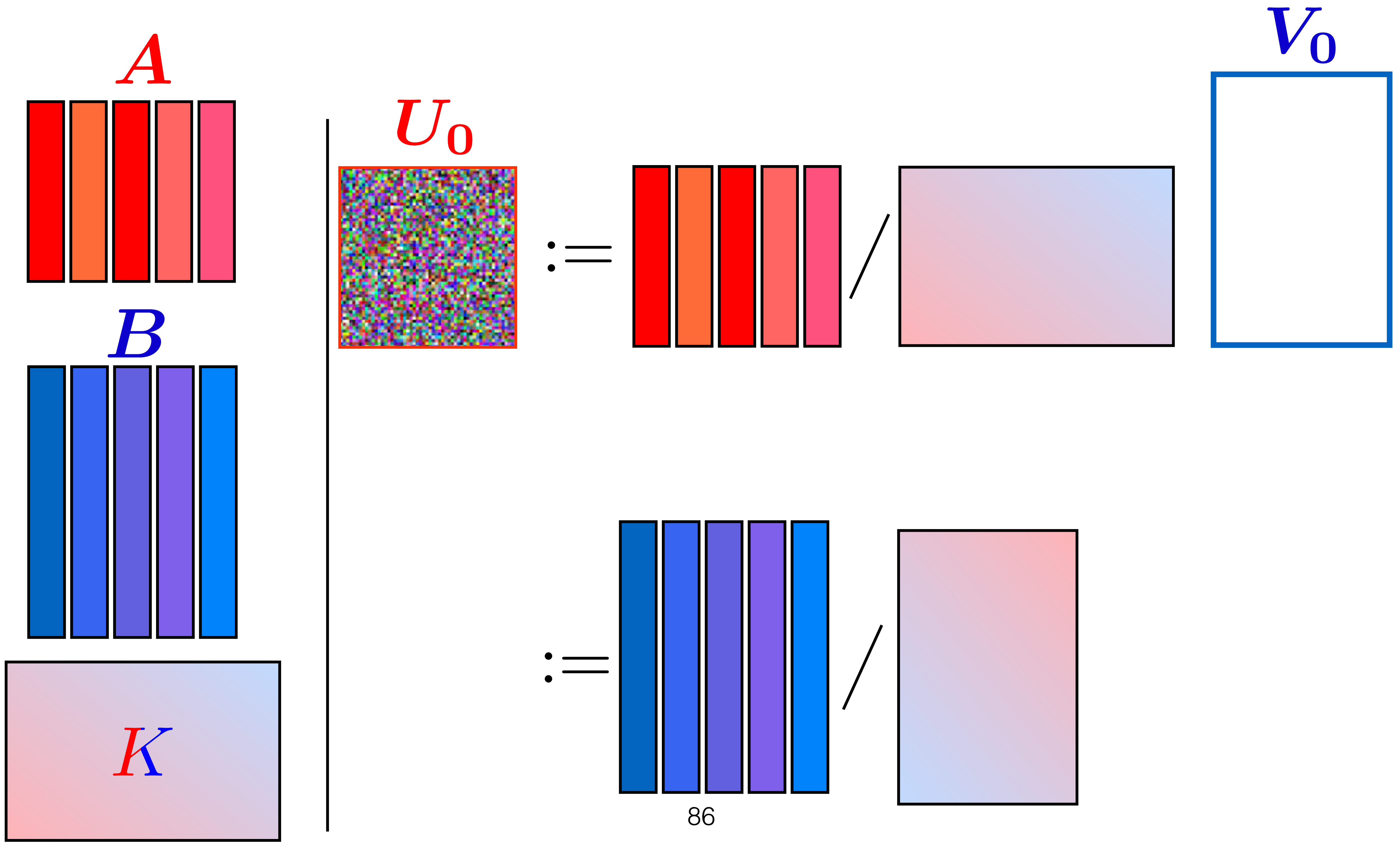

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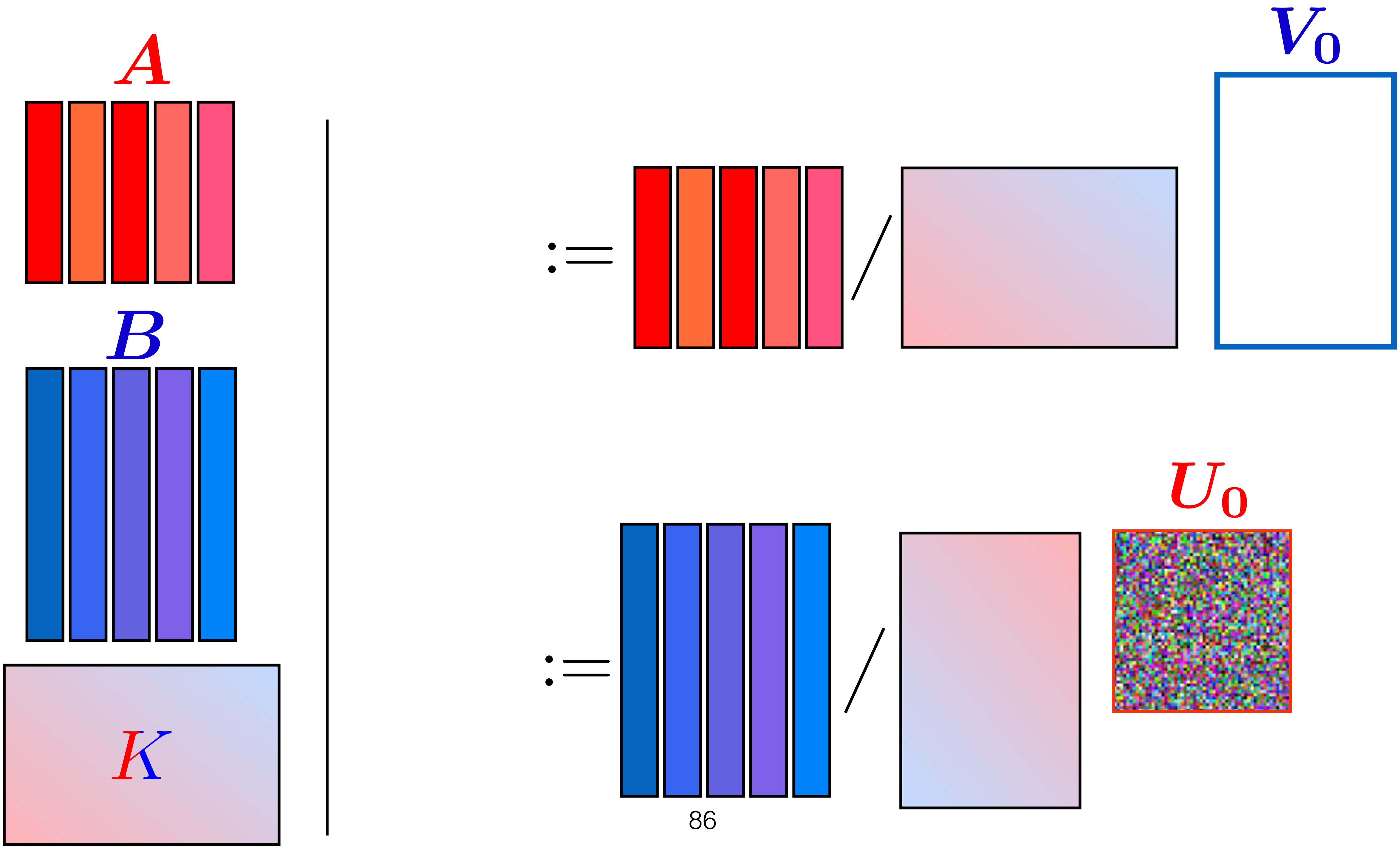

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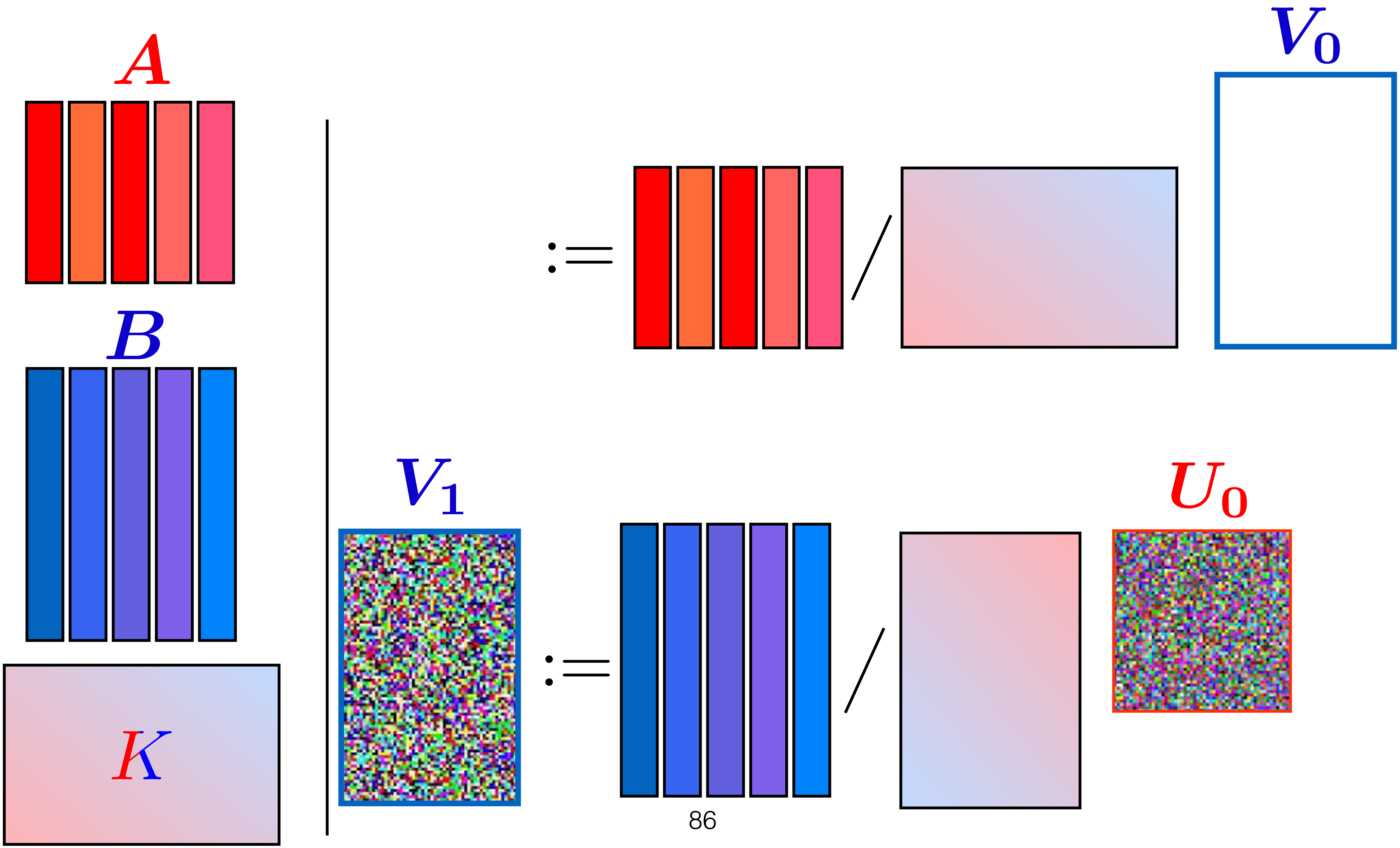

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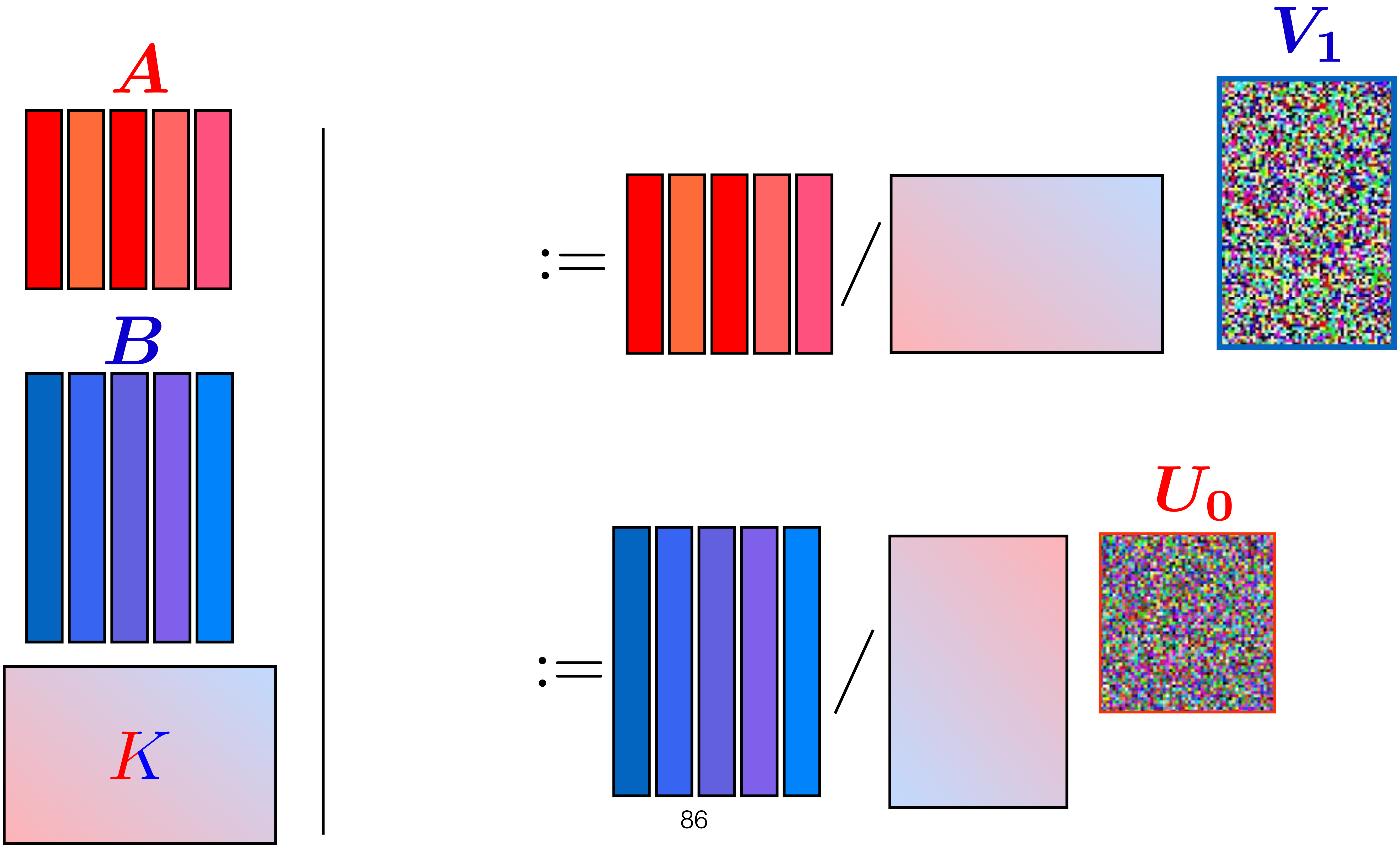
- **[Sinkhorn'64]** with *matrix* fixed-point iterations



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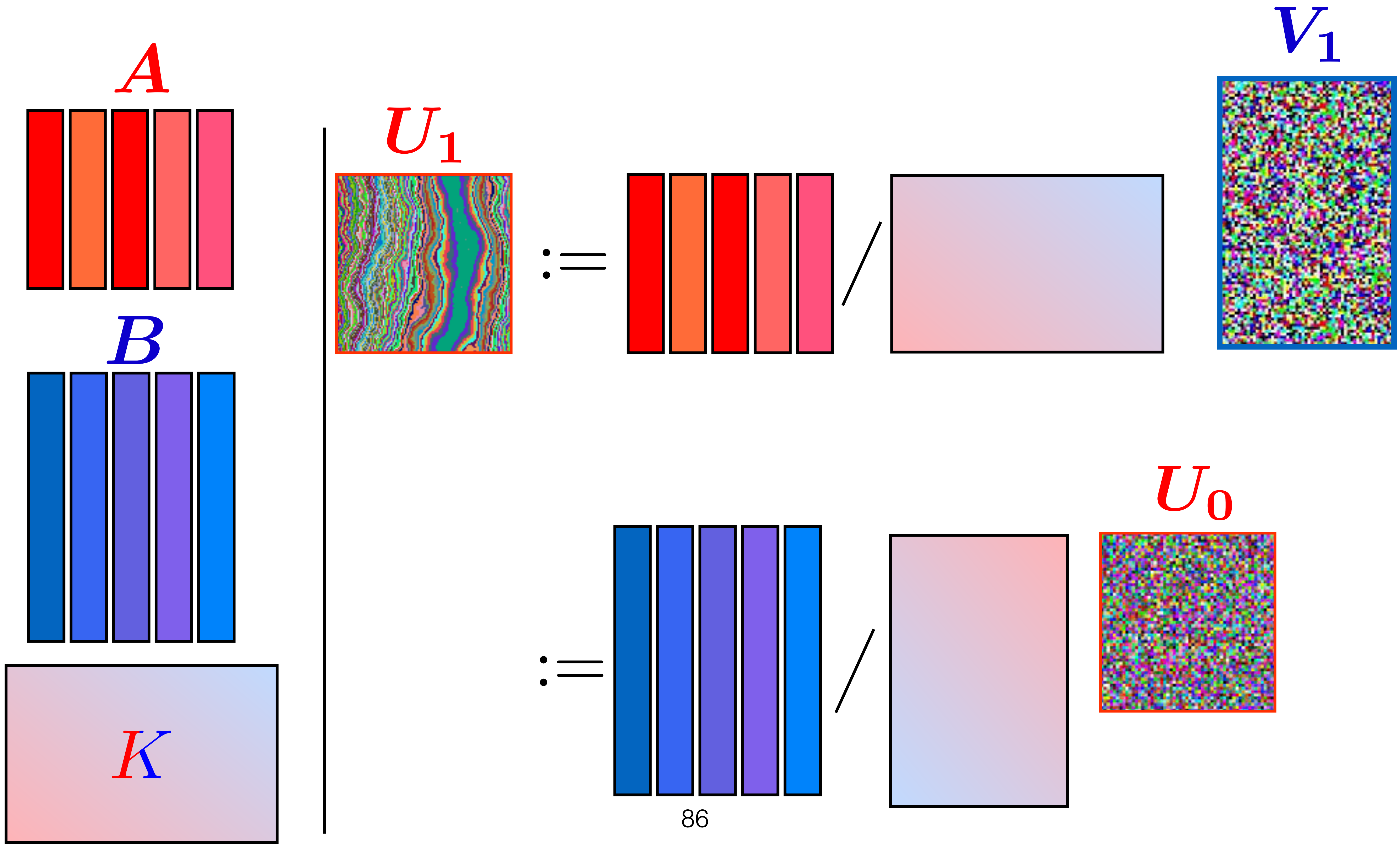

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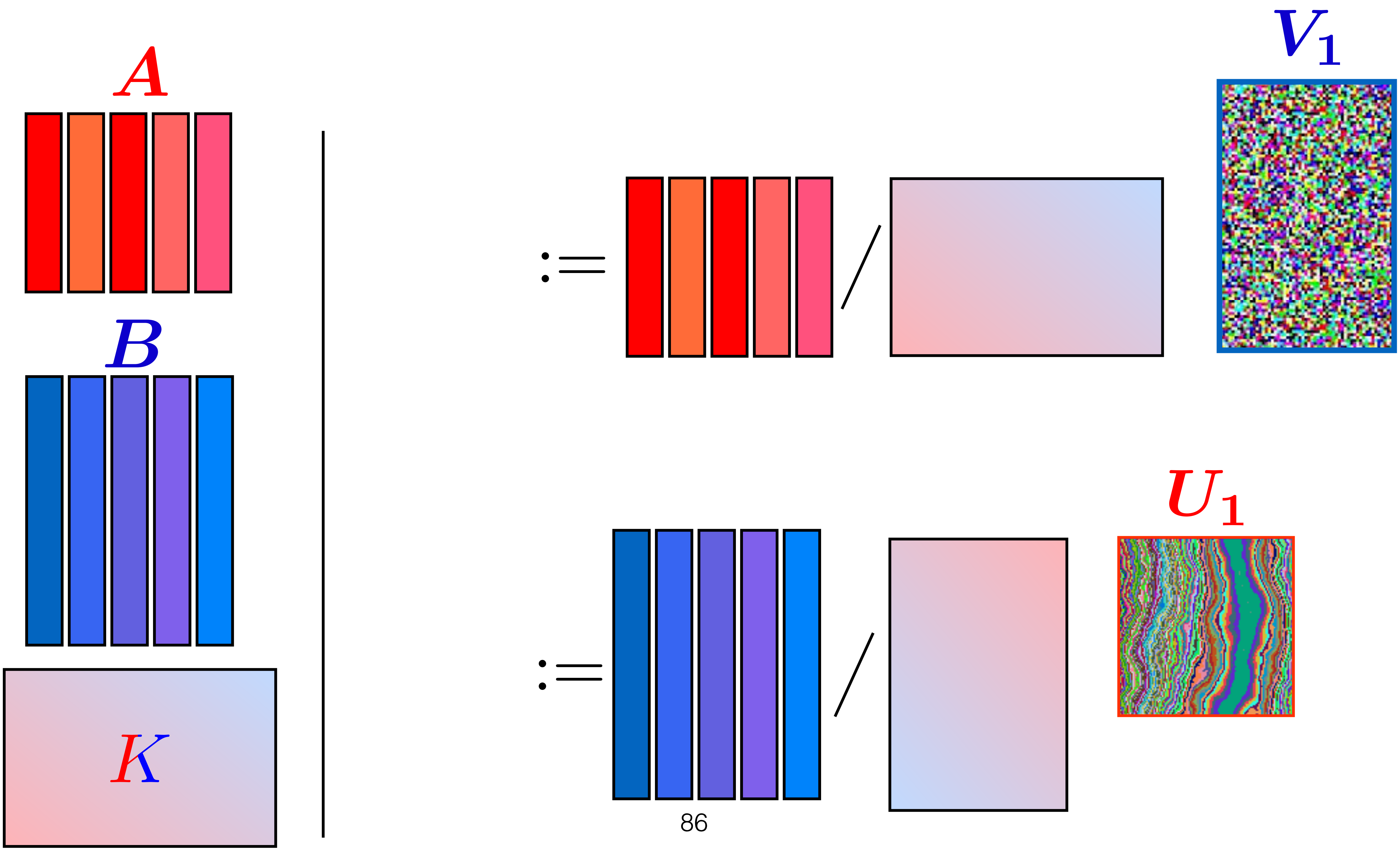

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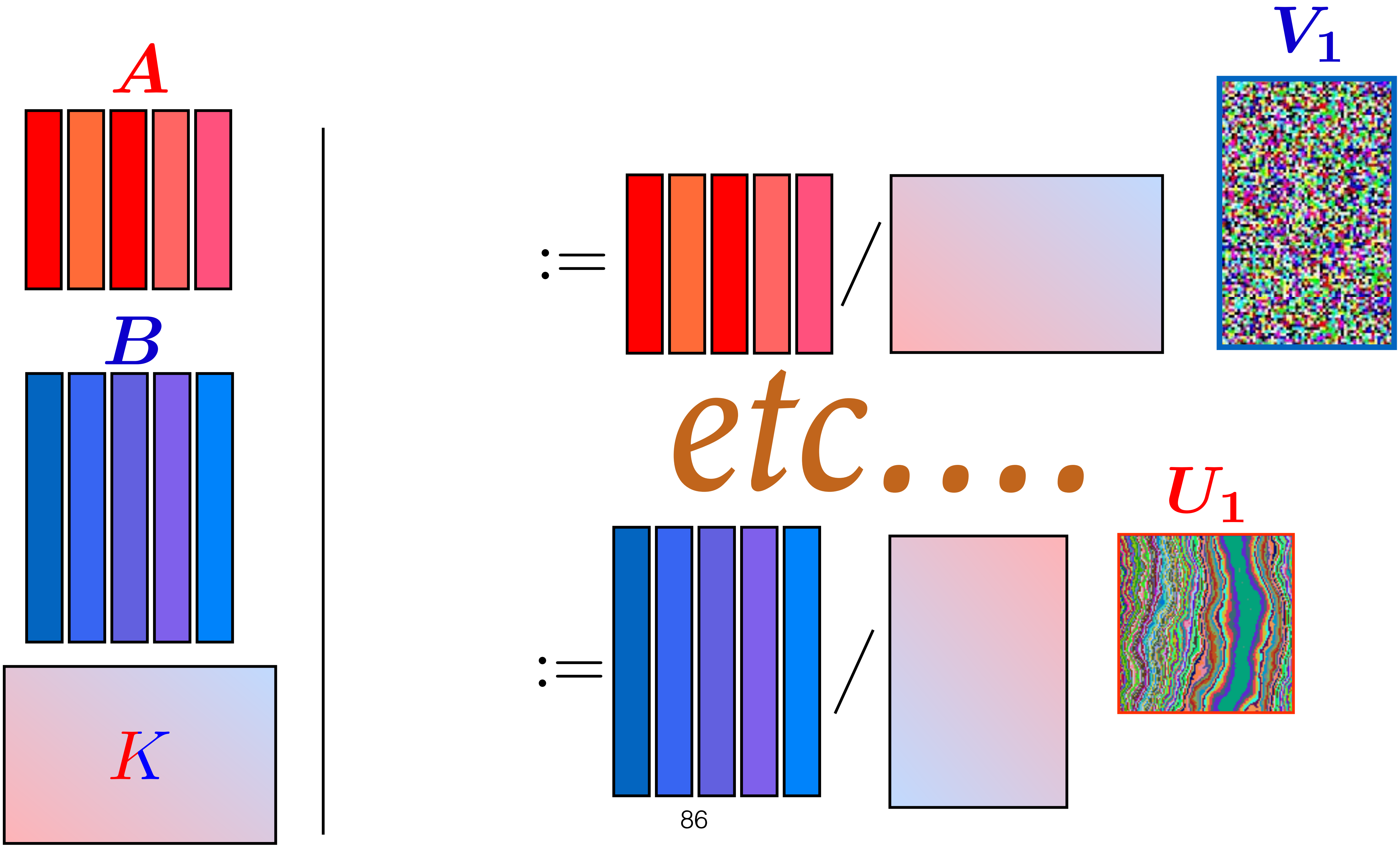
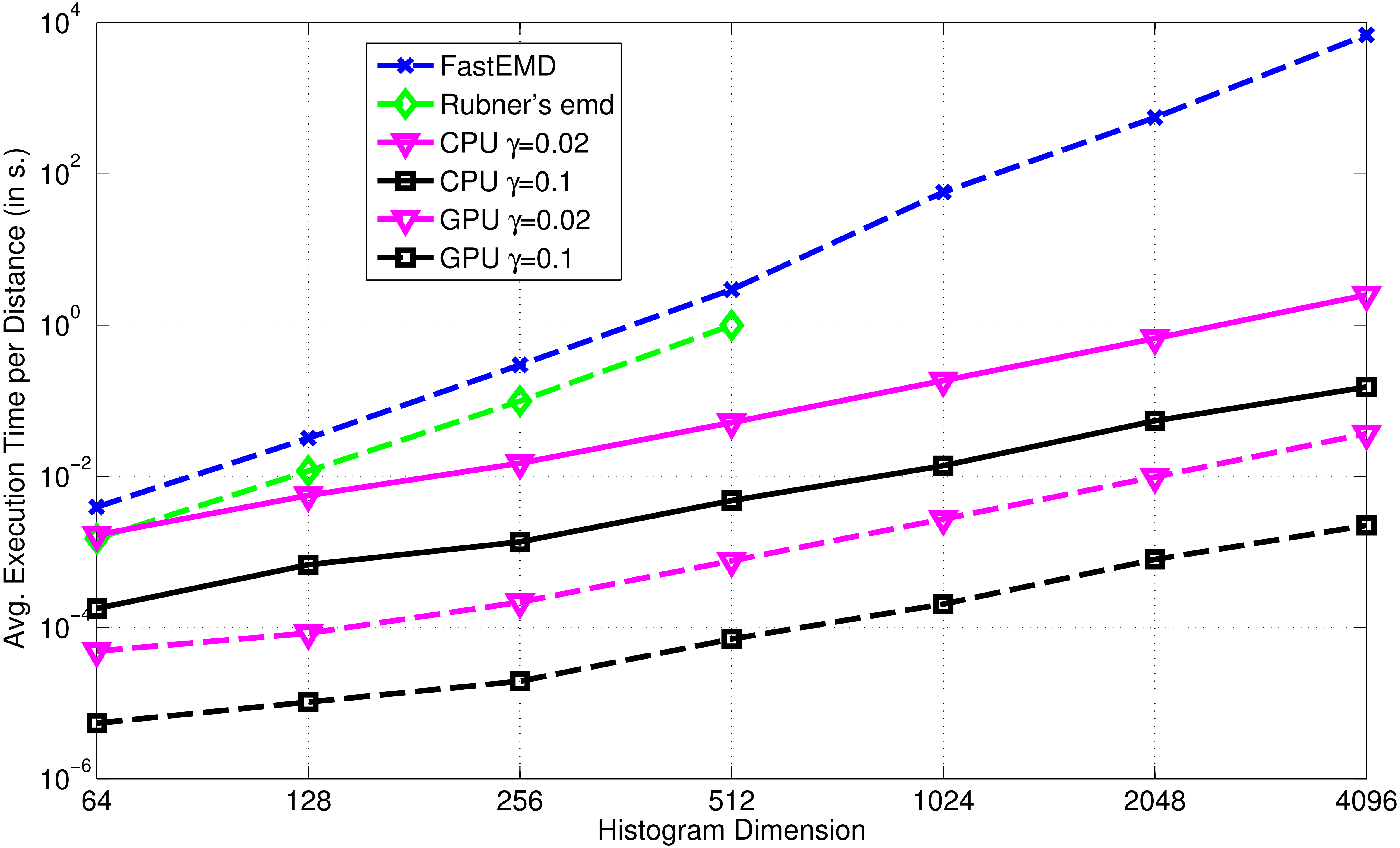


Very Fast EMD Approx. Solver



Note. $(\Omega, \boldsymbol{D})$ is a random graph with shortest path metric, histograms sampled uniformly on simplex, Sinkhorn tolerance 10^{-2}.

Very Fast EMD Approx. Solver

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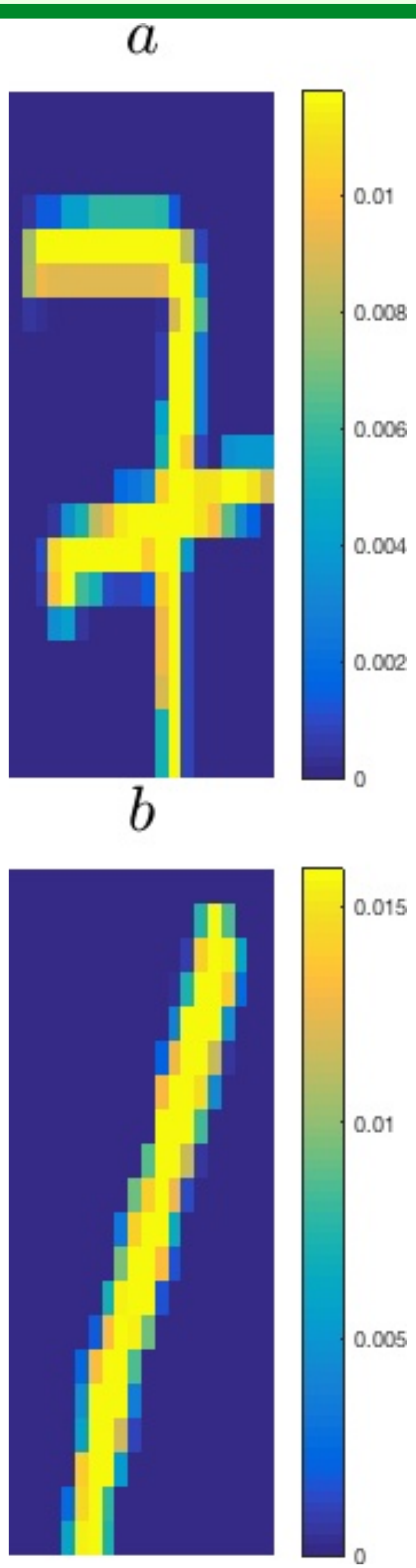
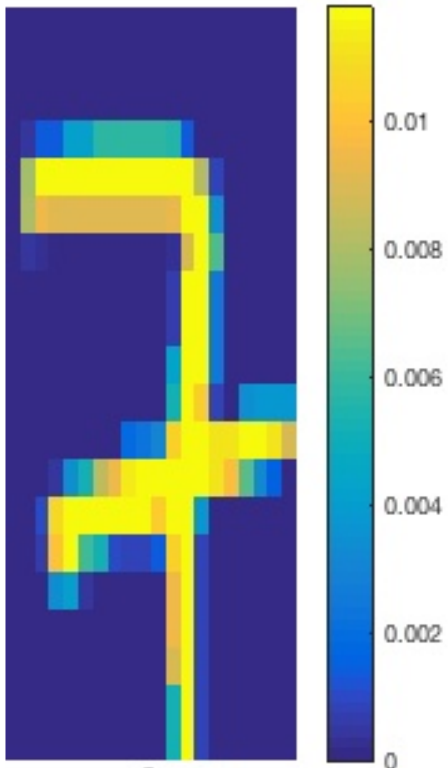
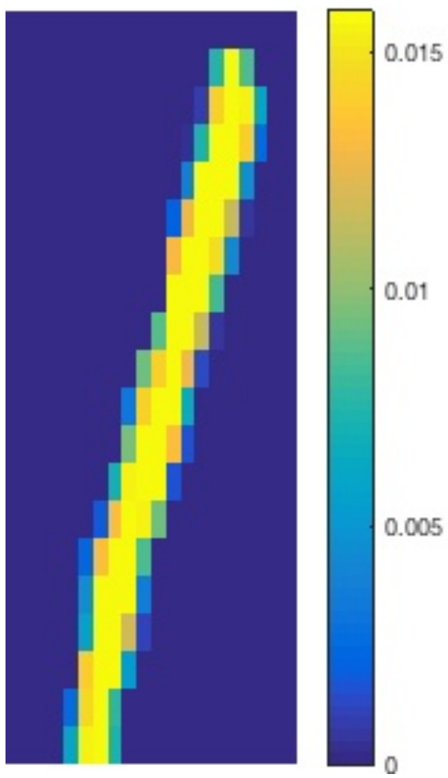


Very Fast EMD Approx. Solver

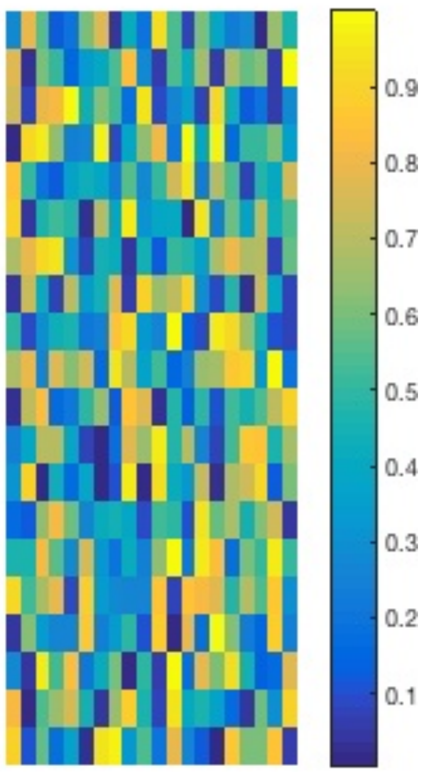
a



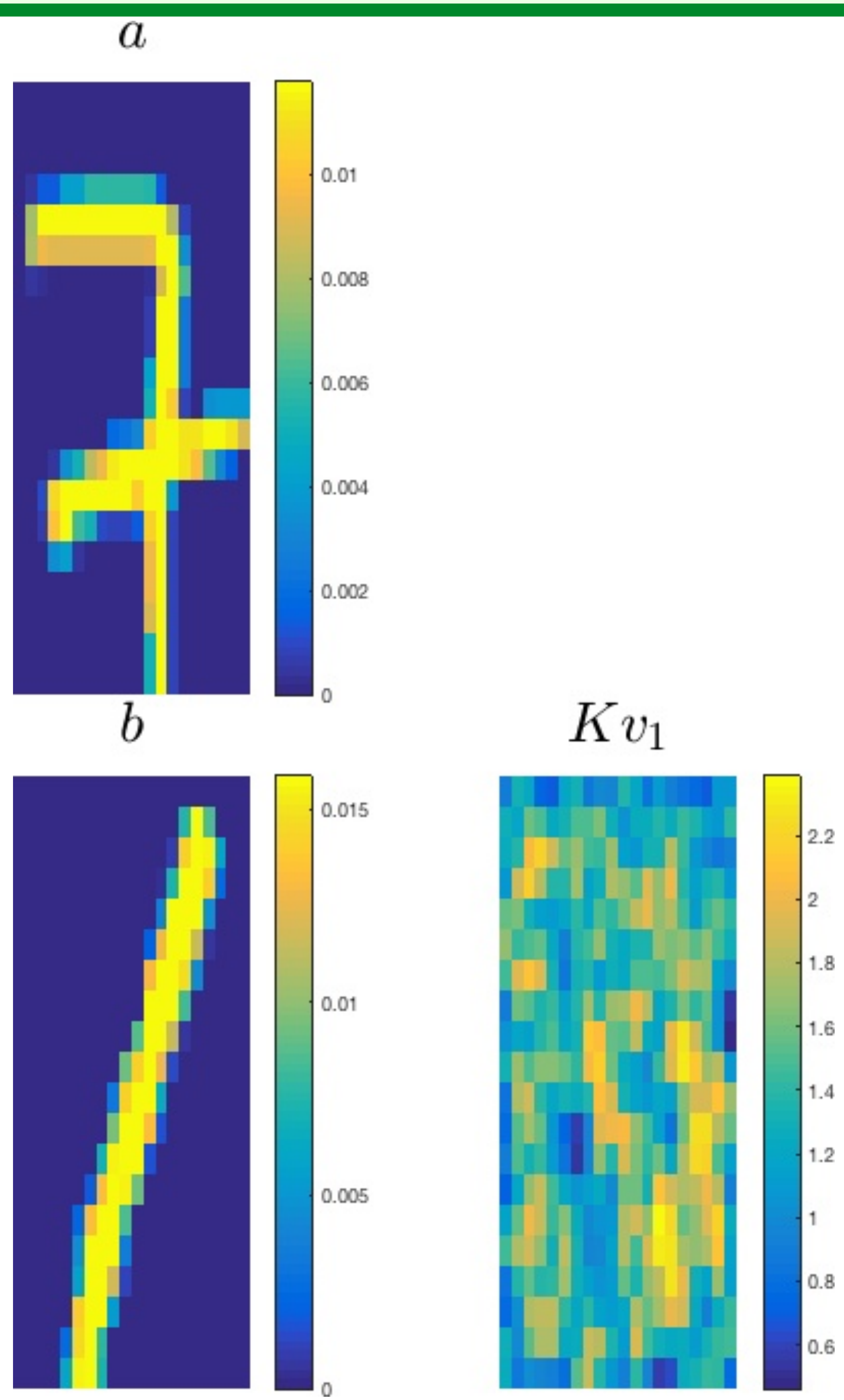
b



$v_1 \leftarrow \text{noise}$



Very Fast EMD Approx. Solver



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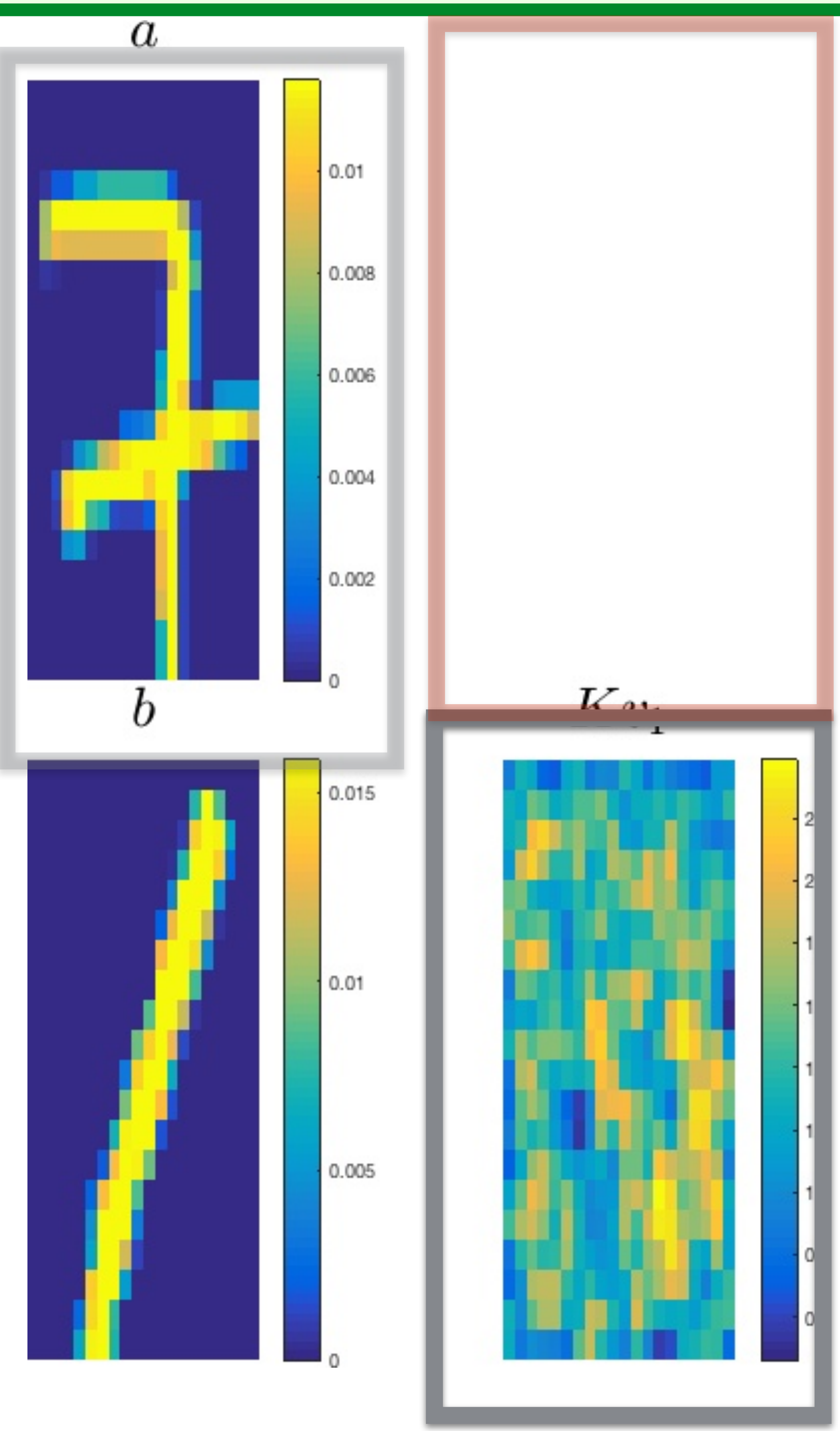

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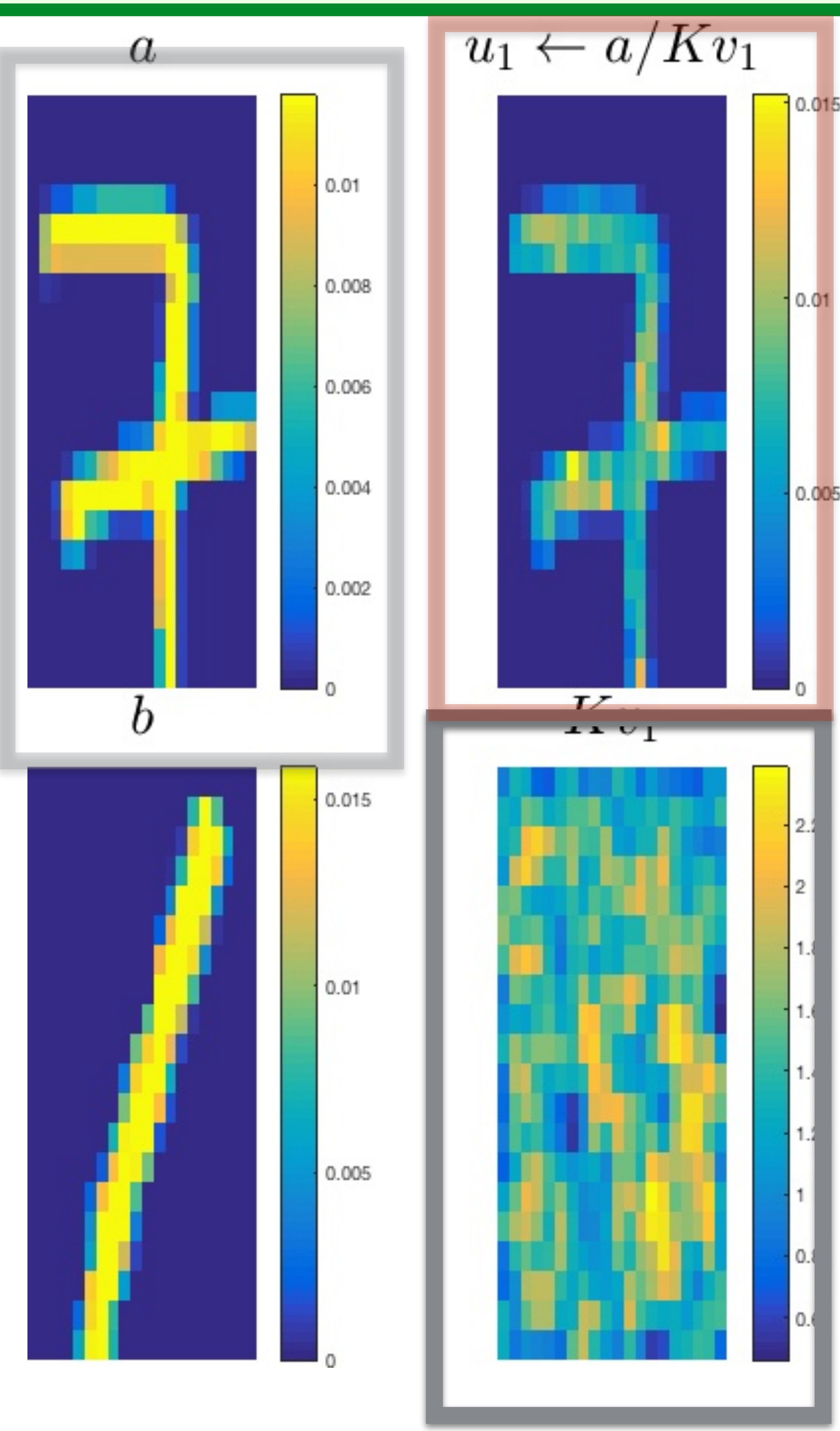
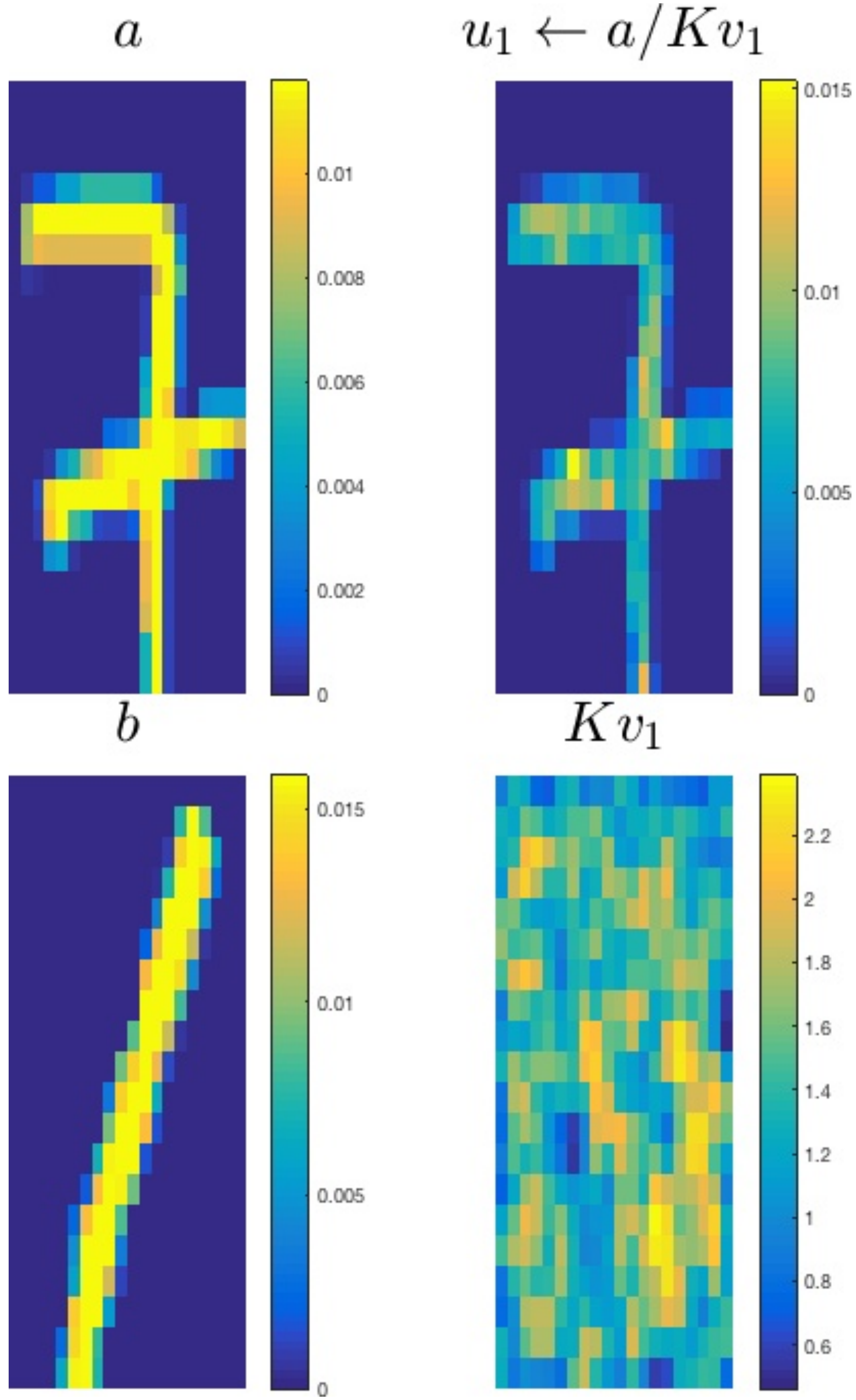
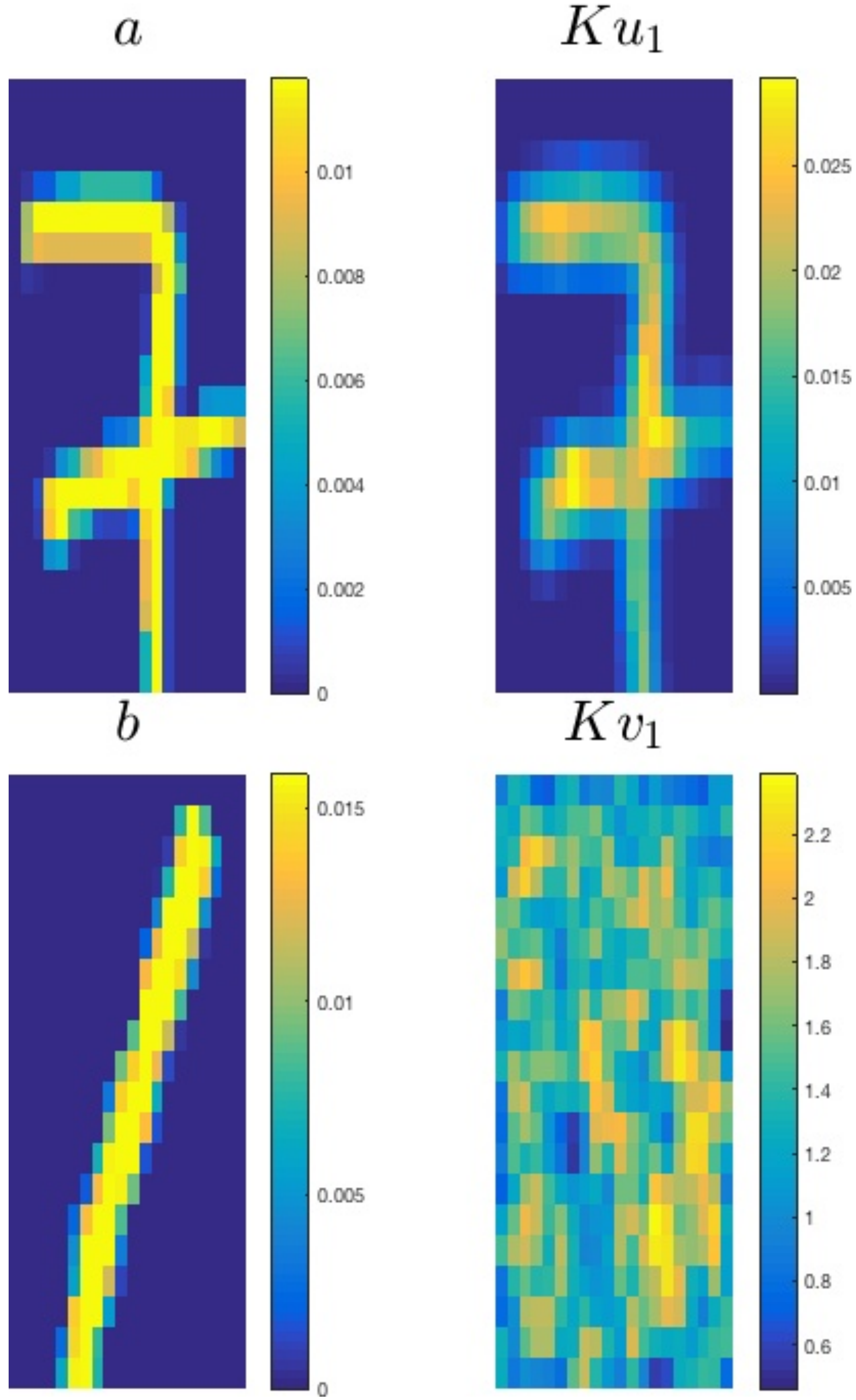


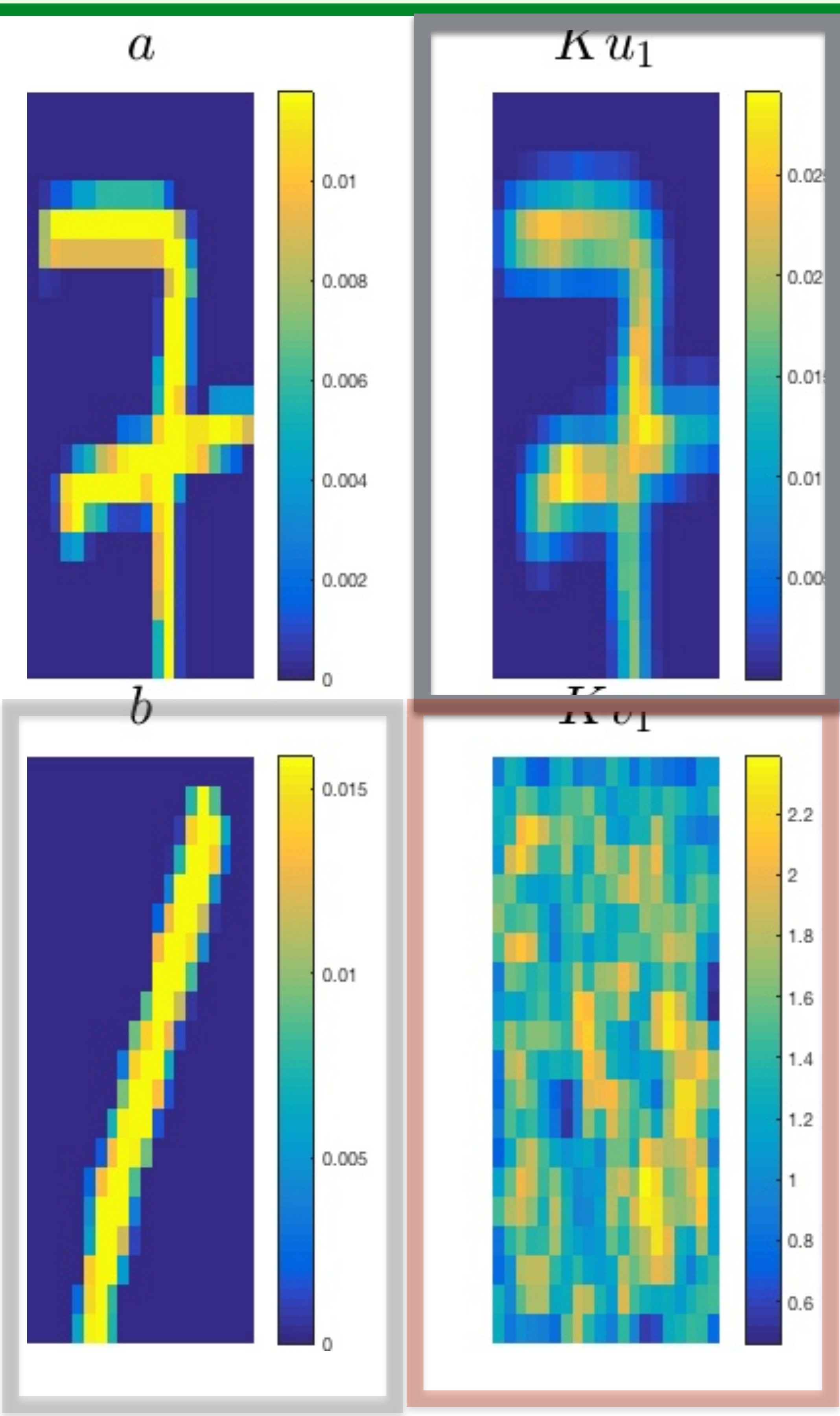
Very Fast EMD Approx. Solver



Very Fast EMD Approx. Solver



Very Fast EMD Approx. Solver



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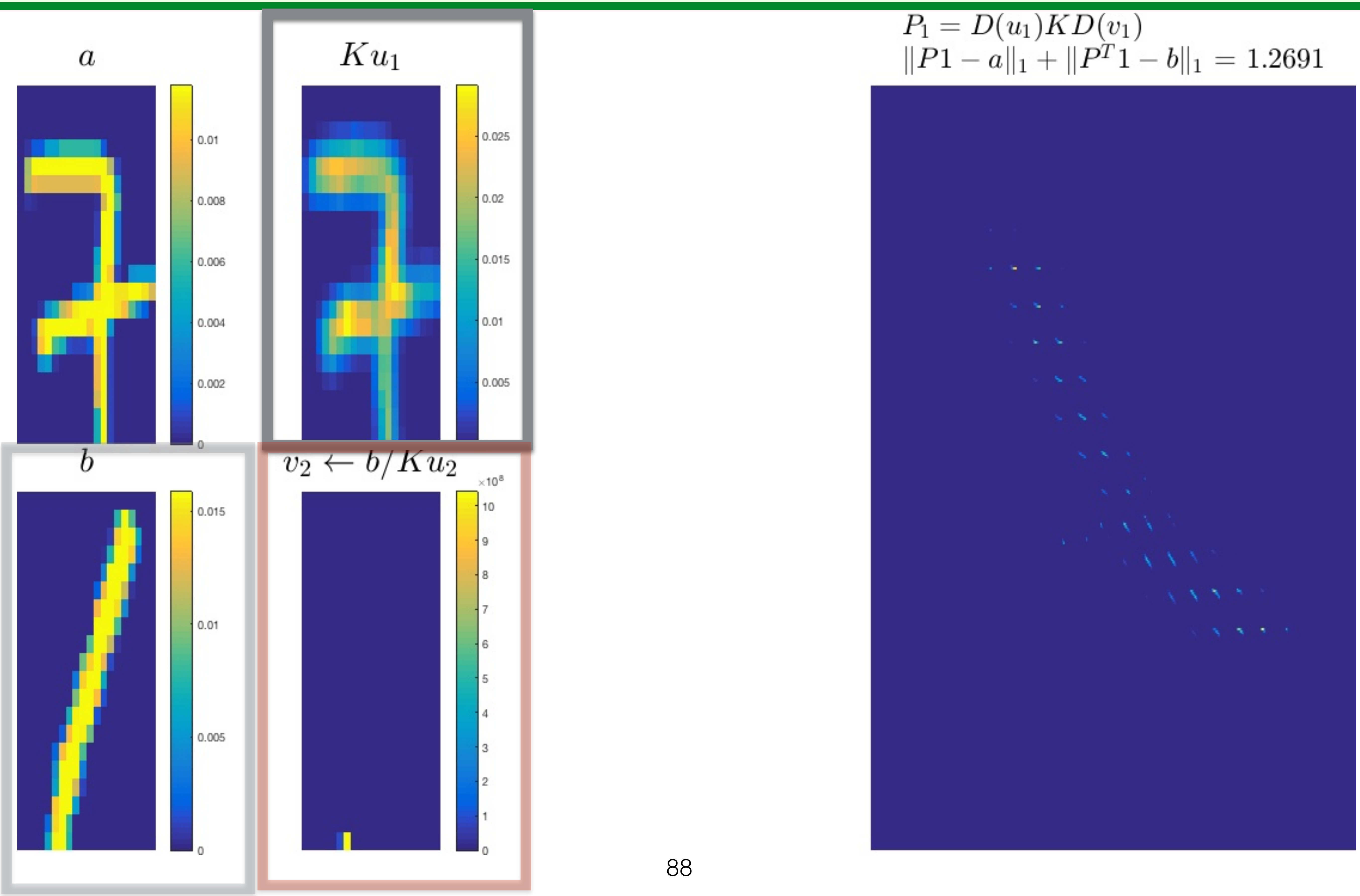

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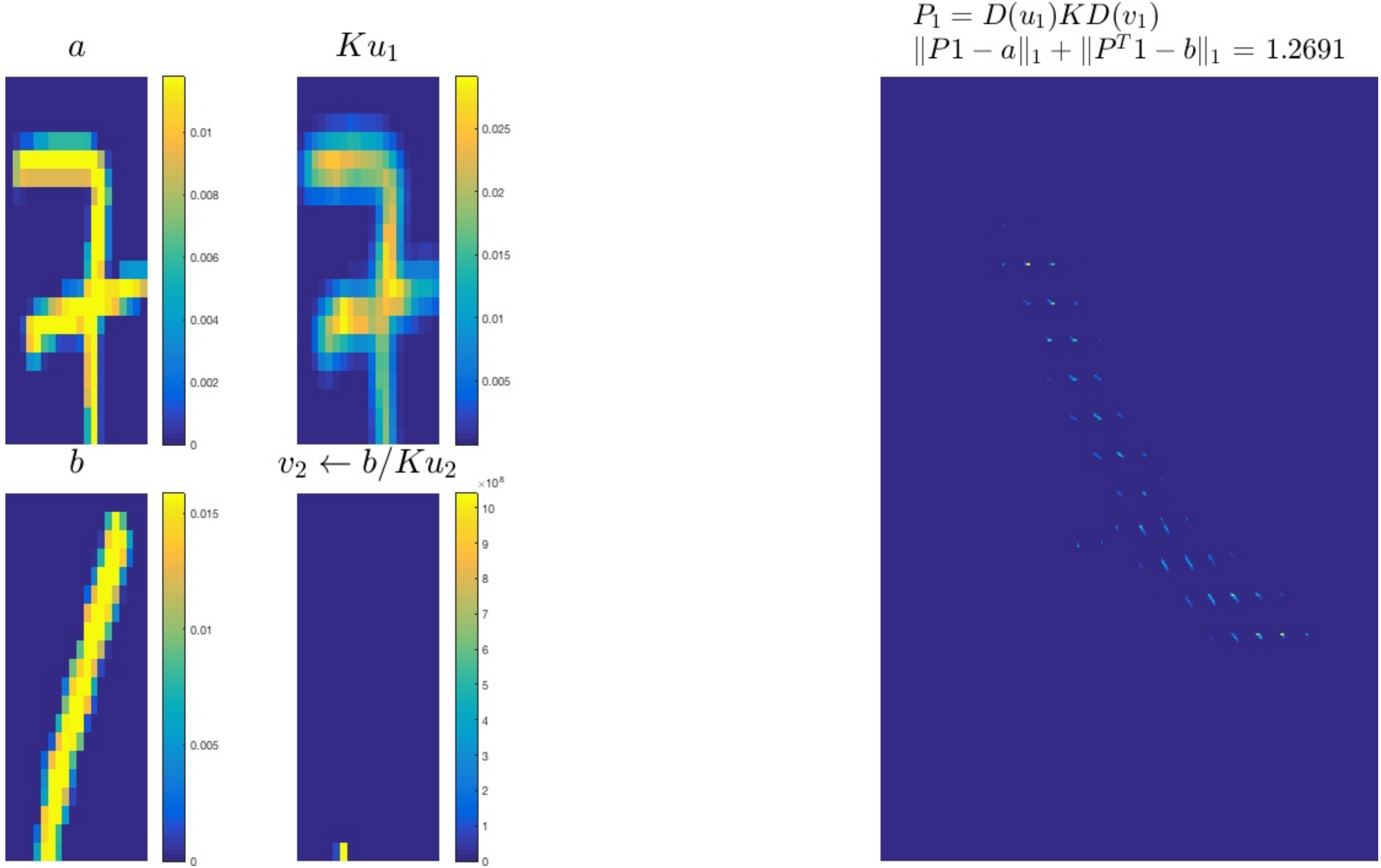

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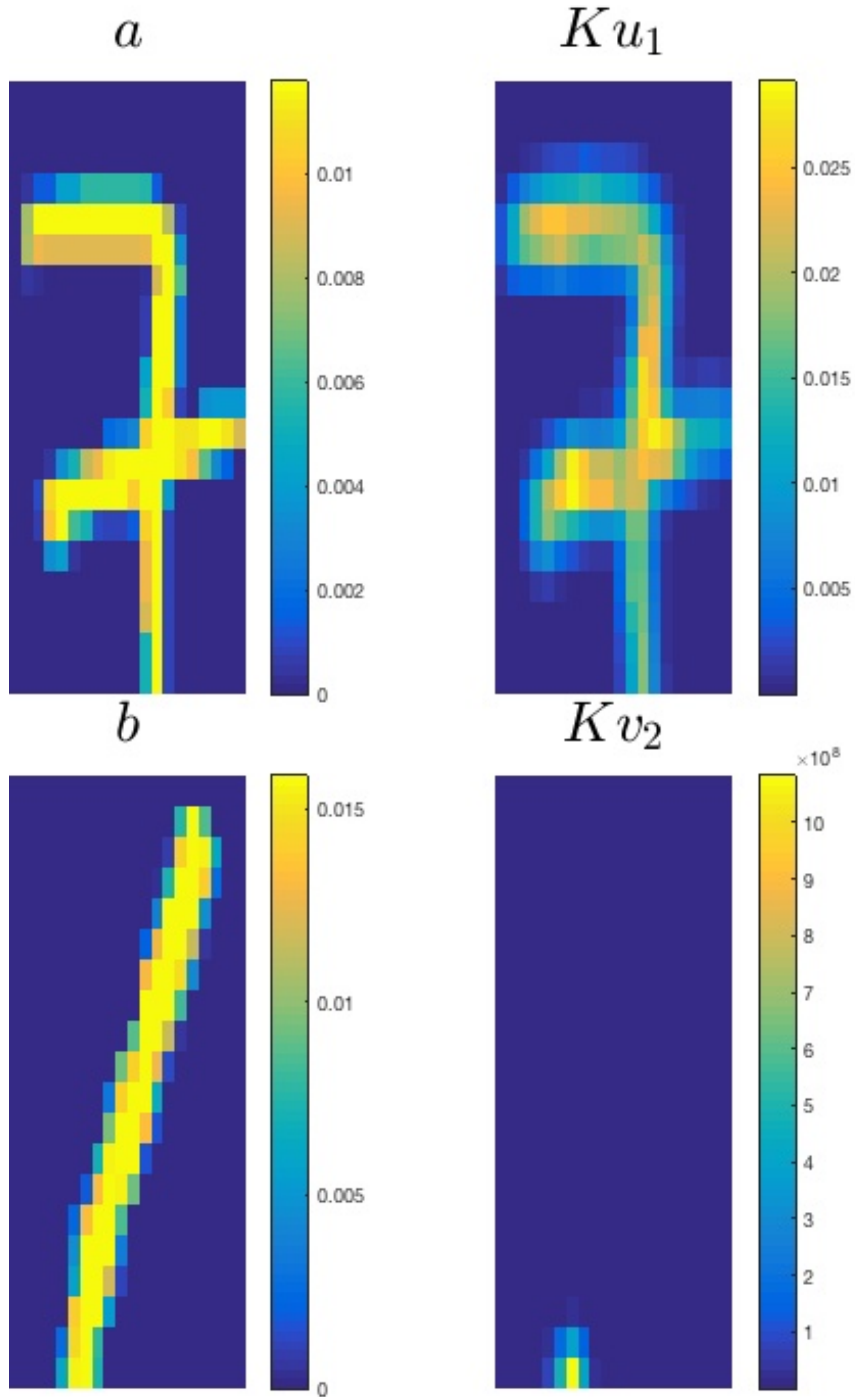

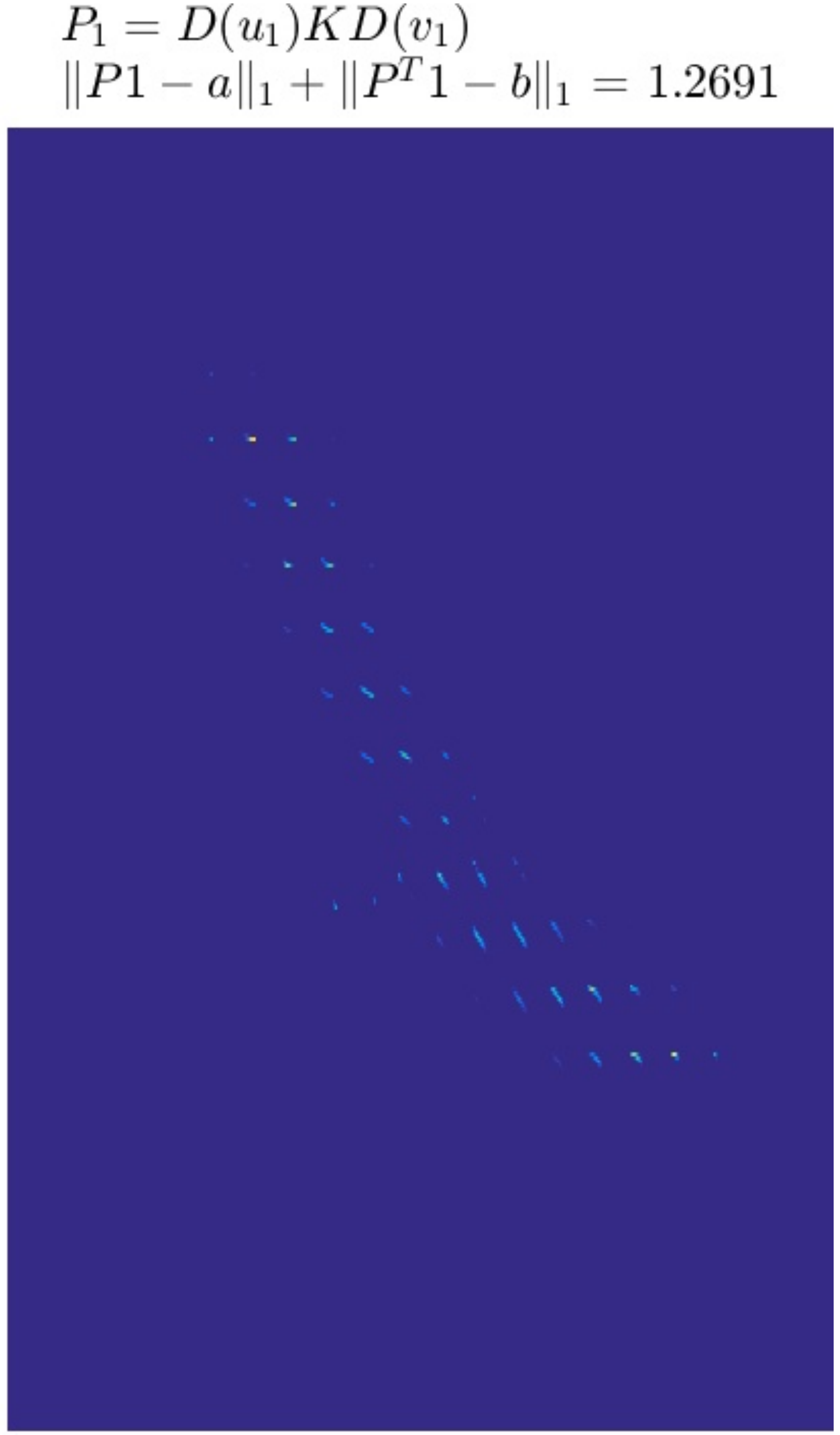

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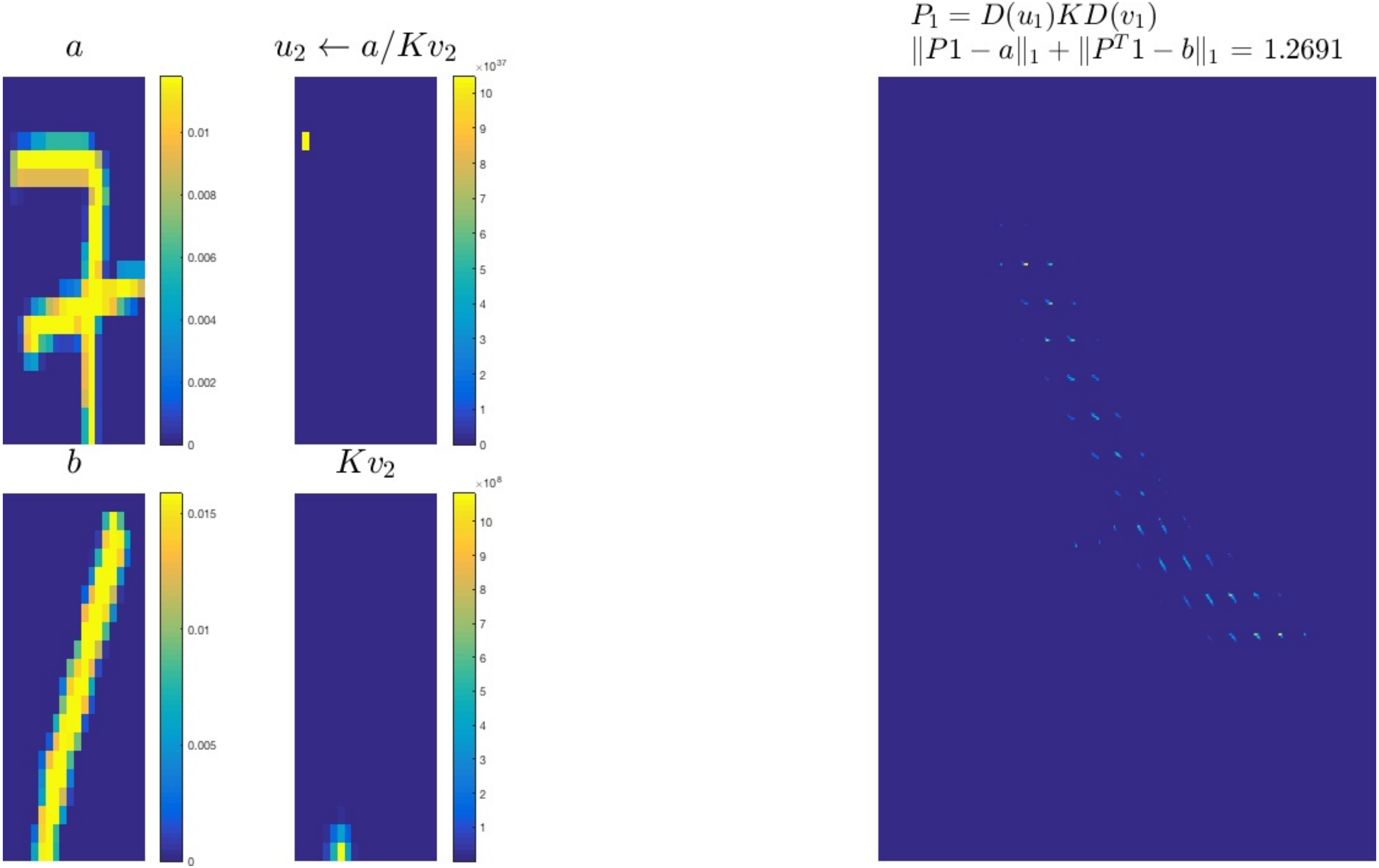
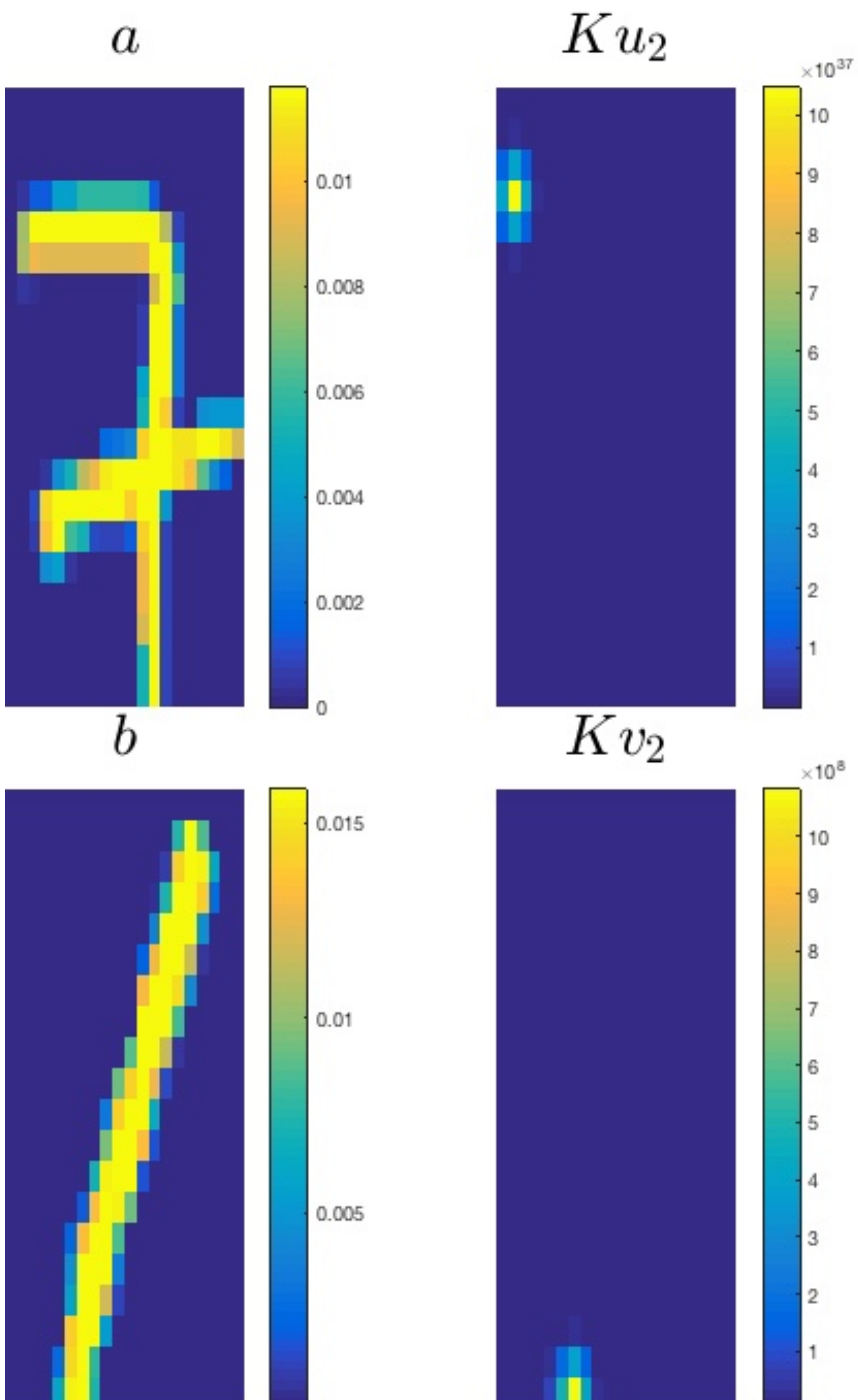


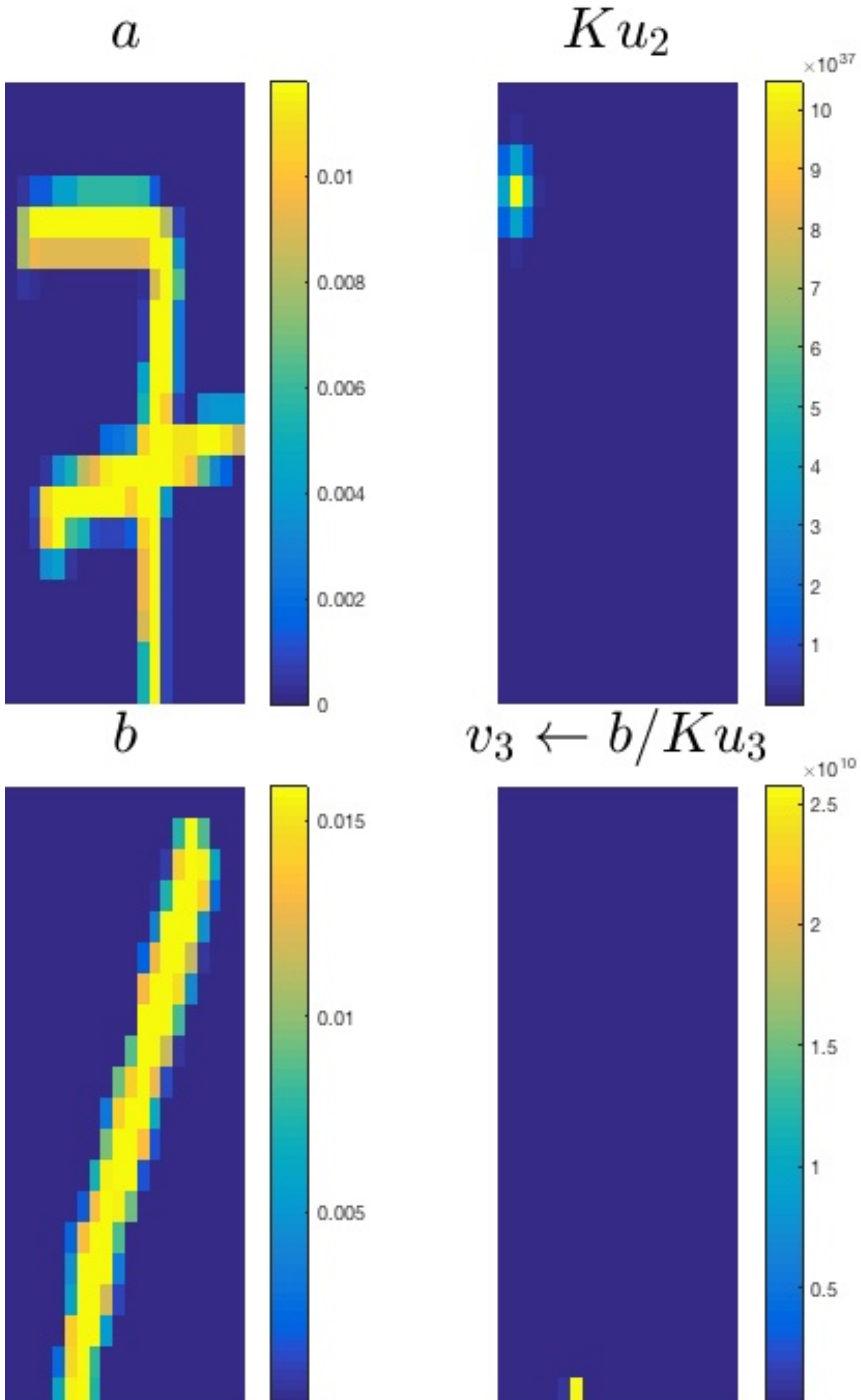
Very Fast EMD Approx. Solver



$P_1 = D(u_1)KD(v_1)$

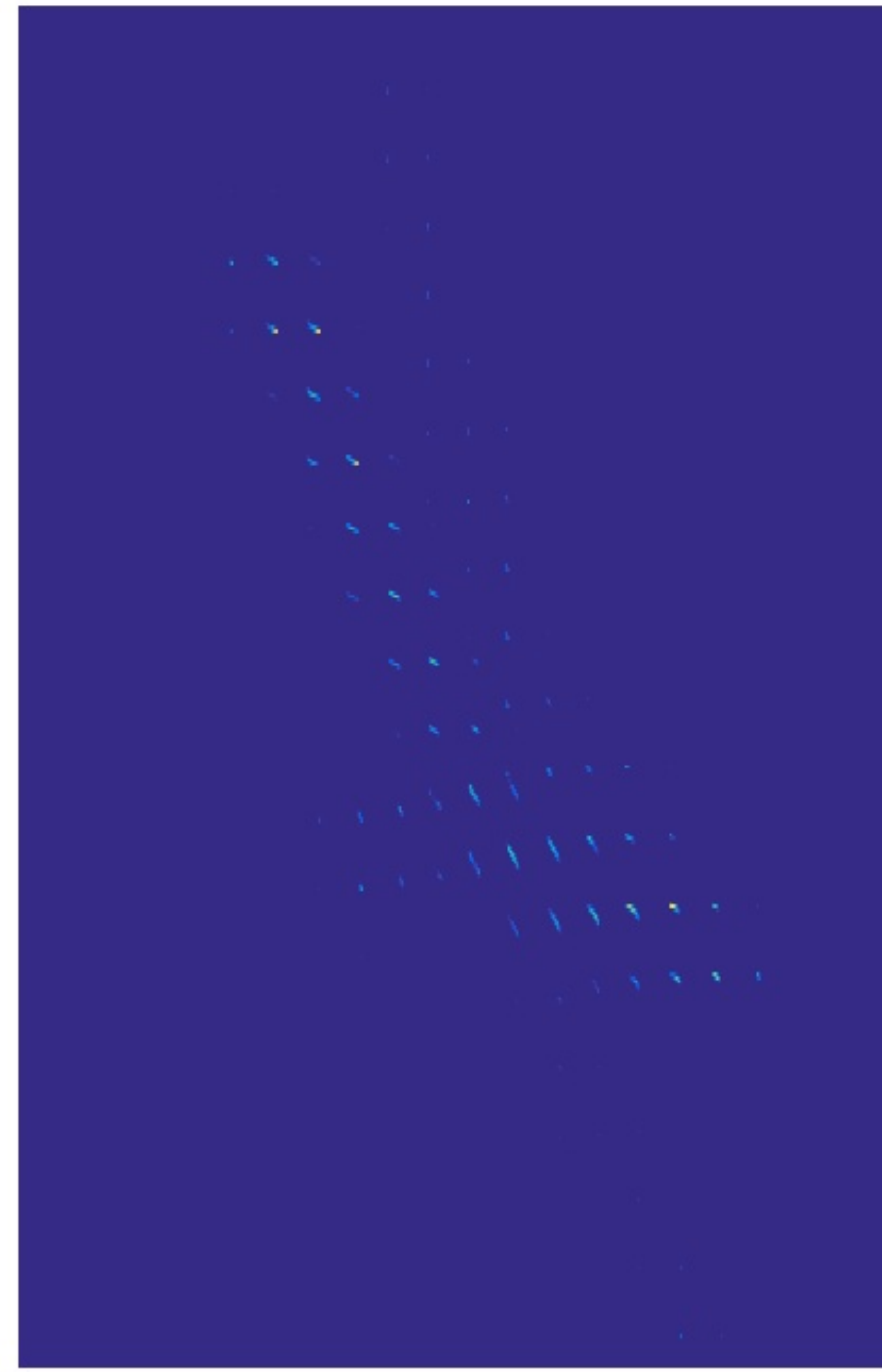
$\|P1 - a\|_1 + \|P^T 1 - b\|_1 = 1.2691$

Very Fast EMD Approx. Solver

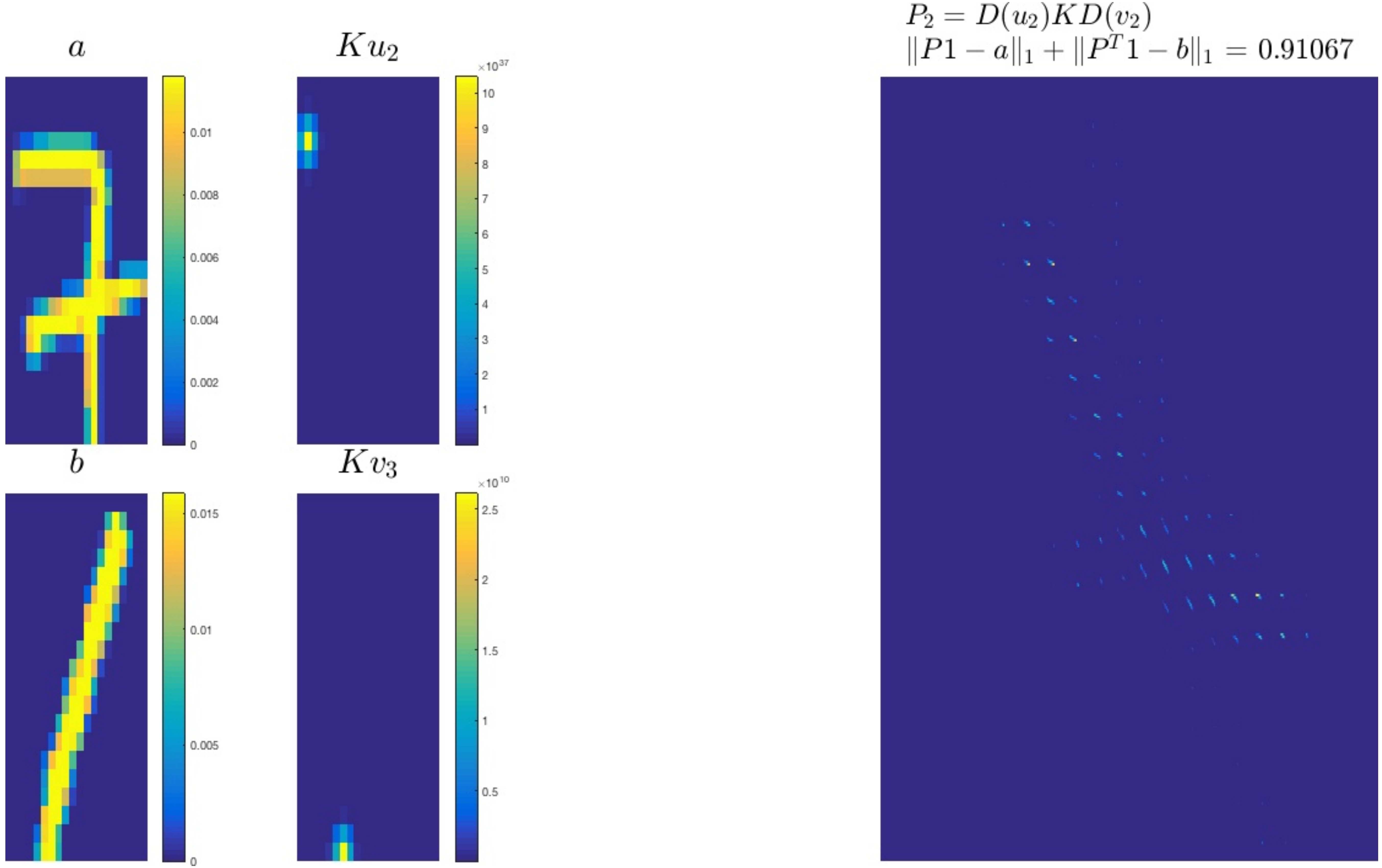


$P_2 = D(u_2)KD(v_2)$

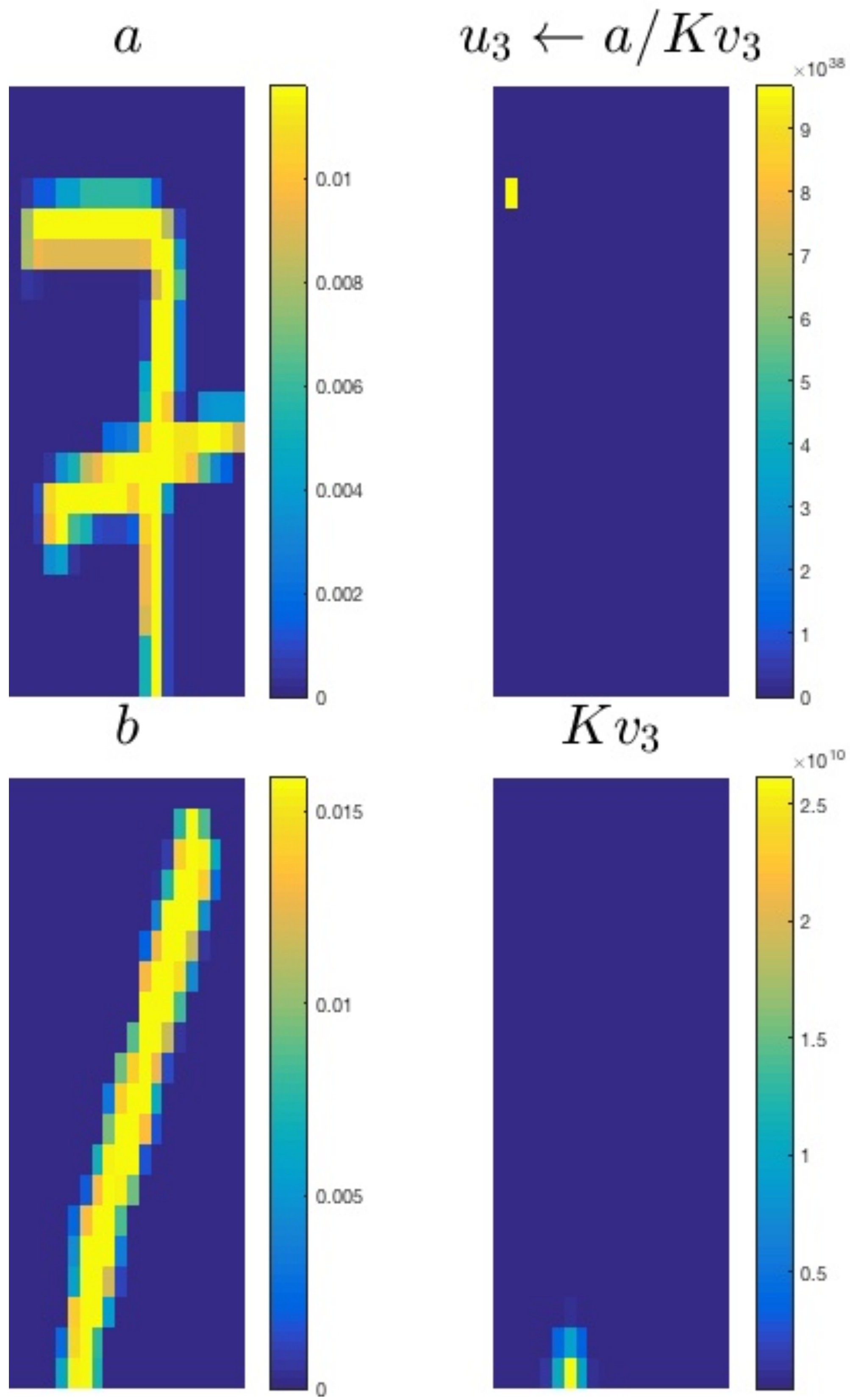
$\|P\mathbb{1} - a\|_1 + \|P^T\mathbb{1} - b\|_1 = 0.91067$

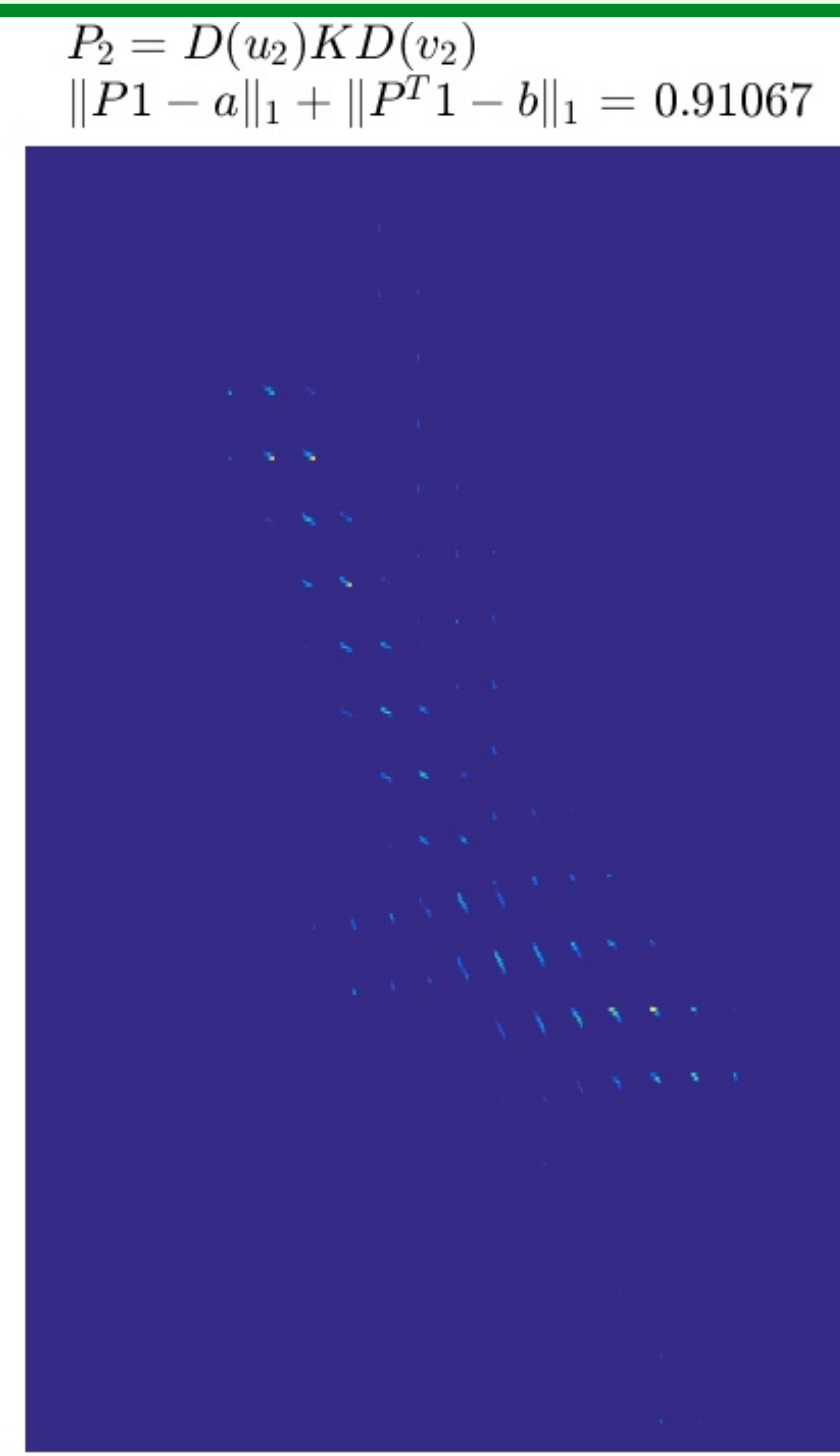


Very Fast EMD Approx. Solver

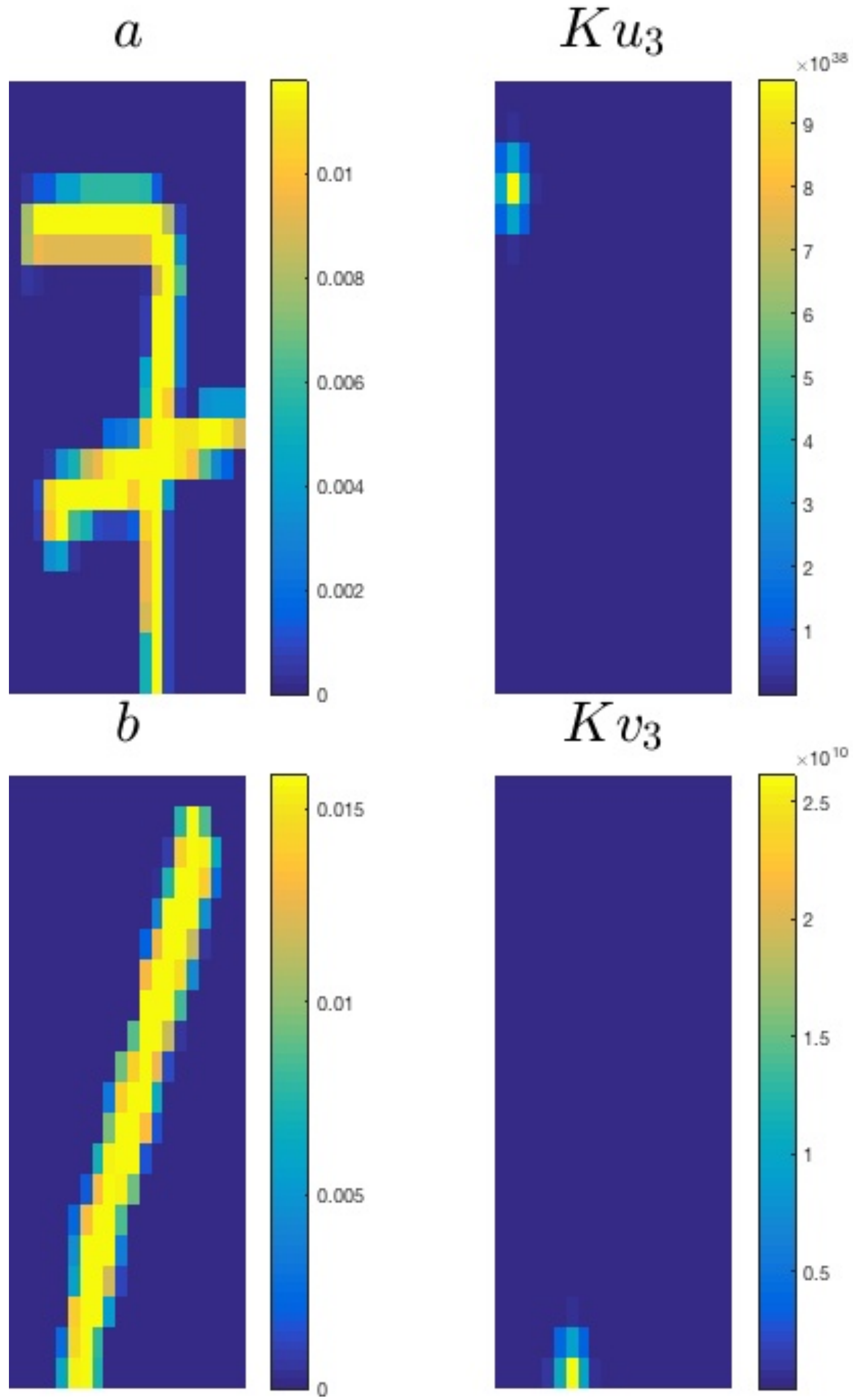


Very Fast EMD Approx. Solver



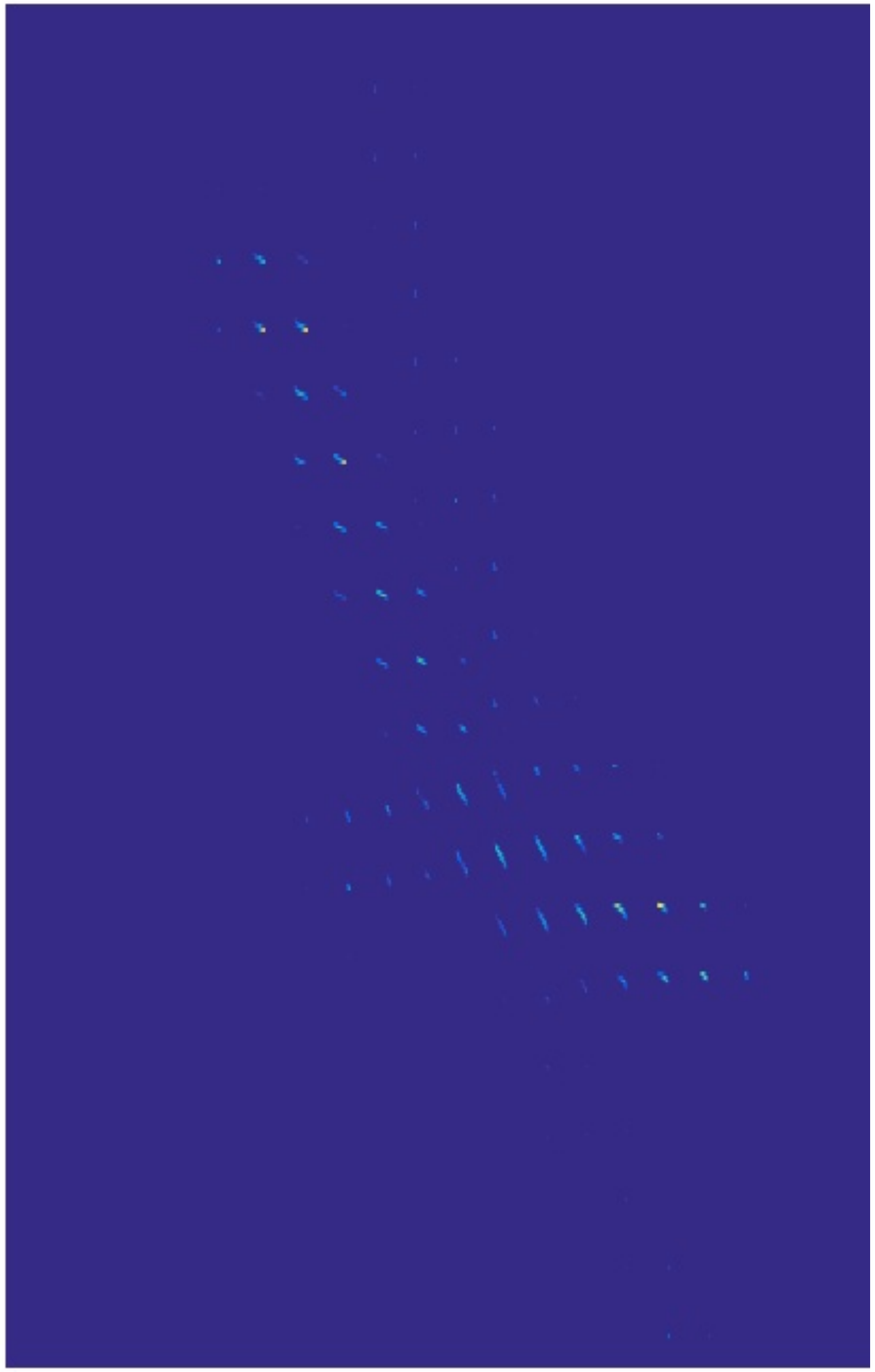


Very Fast EMD Approx. Solver

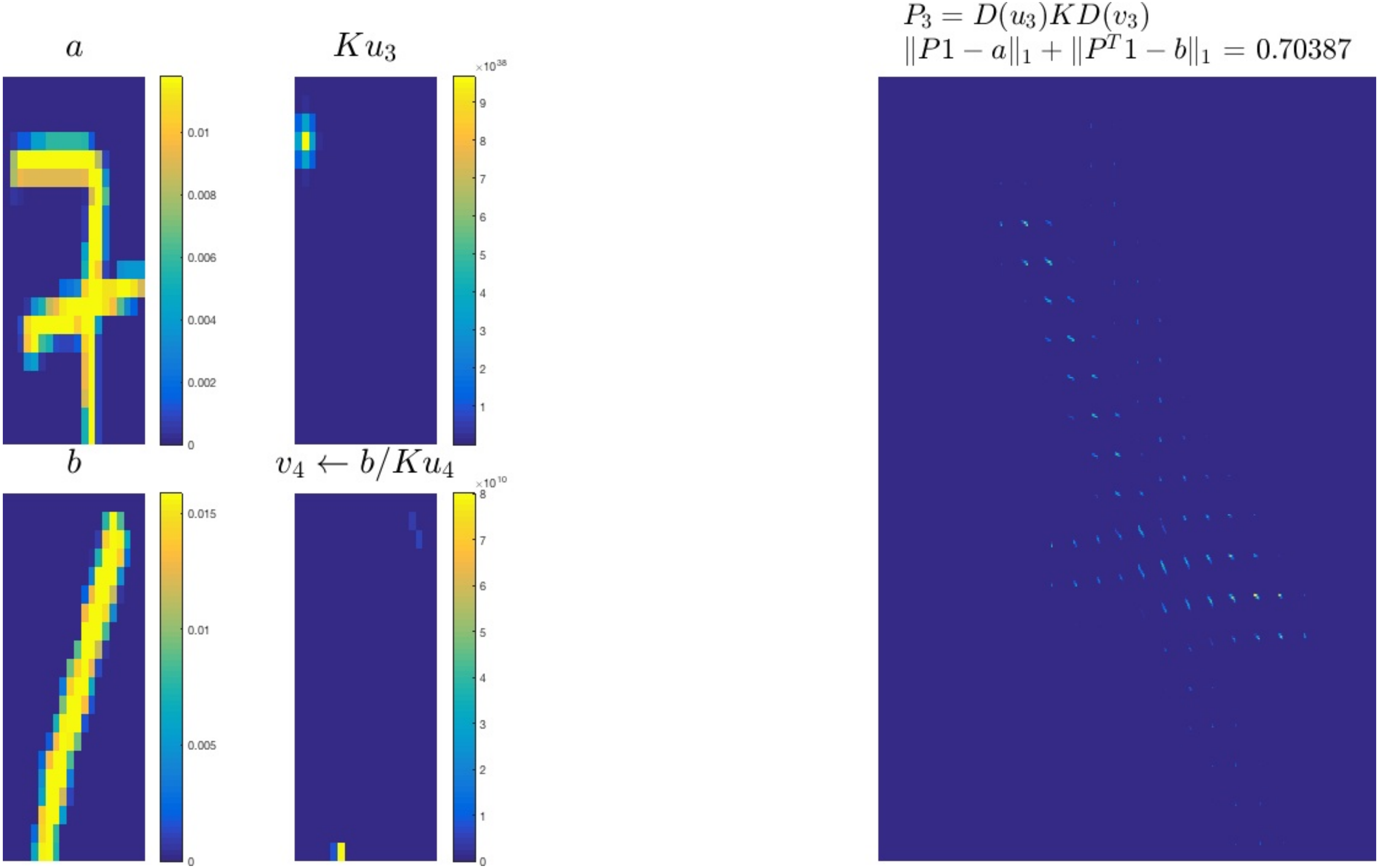


$P_2 = D(u_2)KD(v_2)$

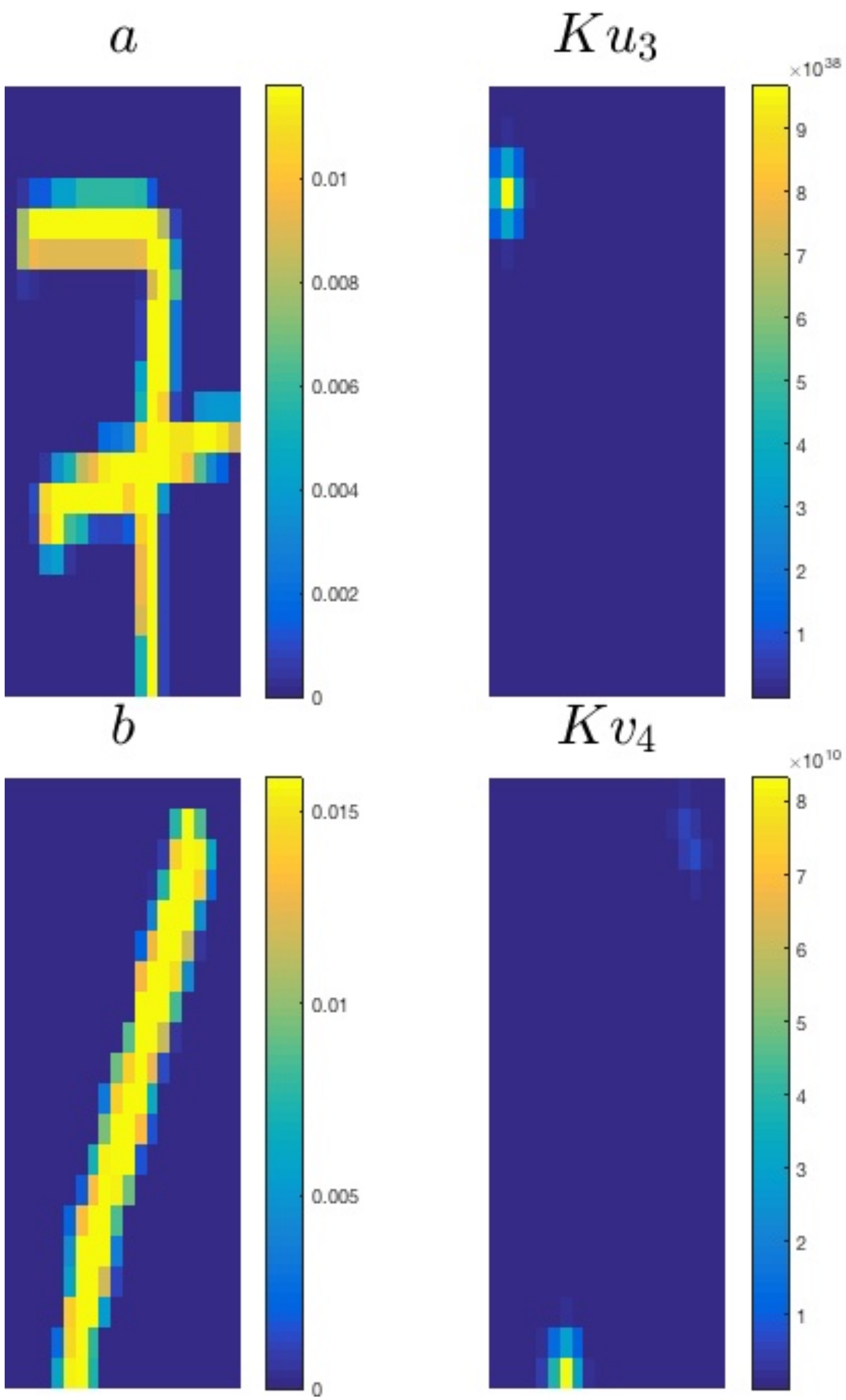
$\|P1 - a\|_1 + \|P^T 1 - b\|_1 = 0.91067$



Very Fast EMD Approx. Solver

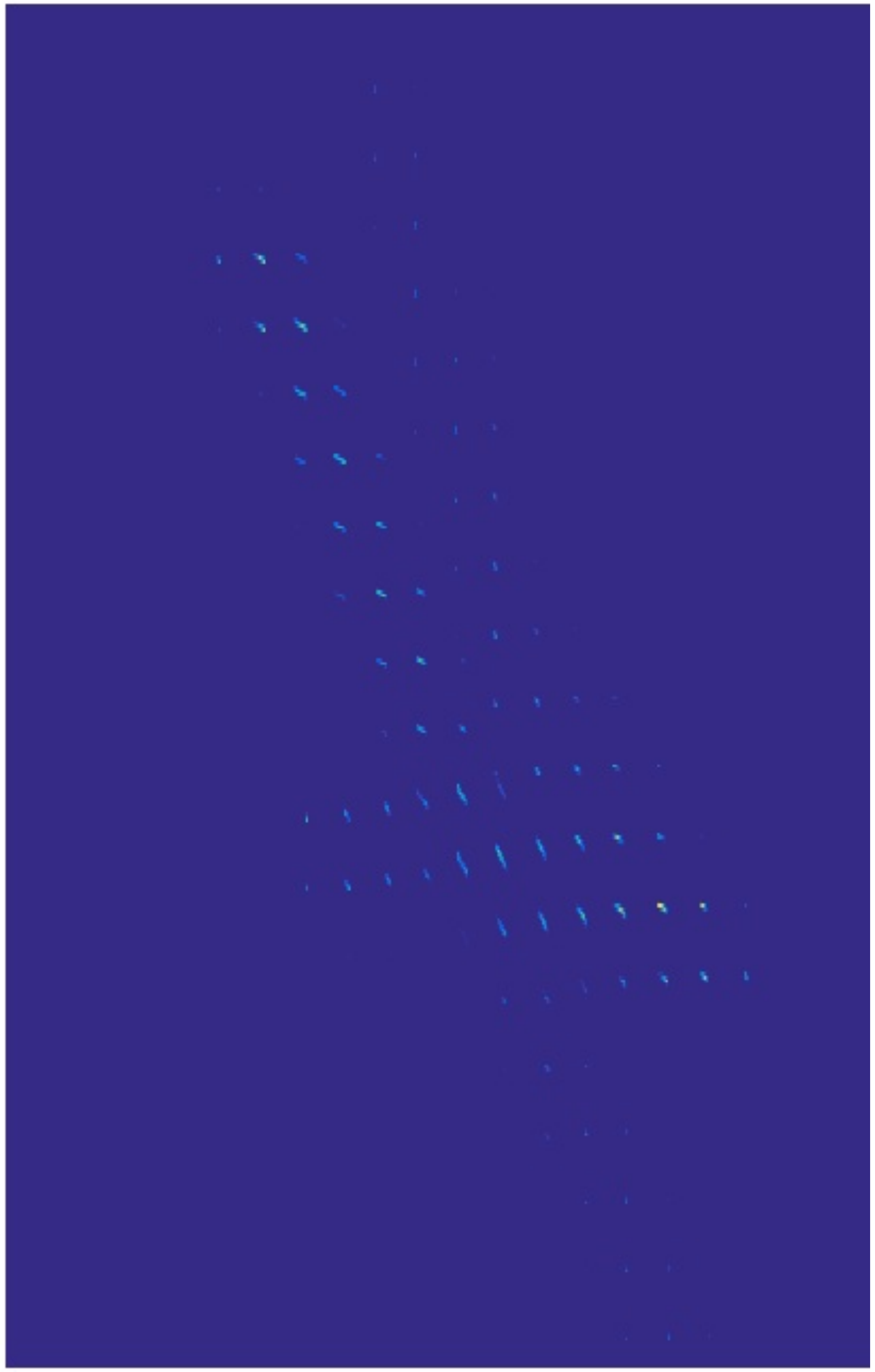


Very Fast EMD Approx. Solver

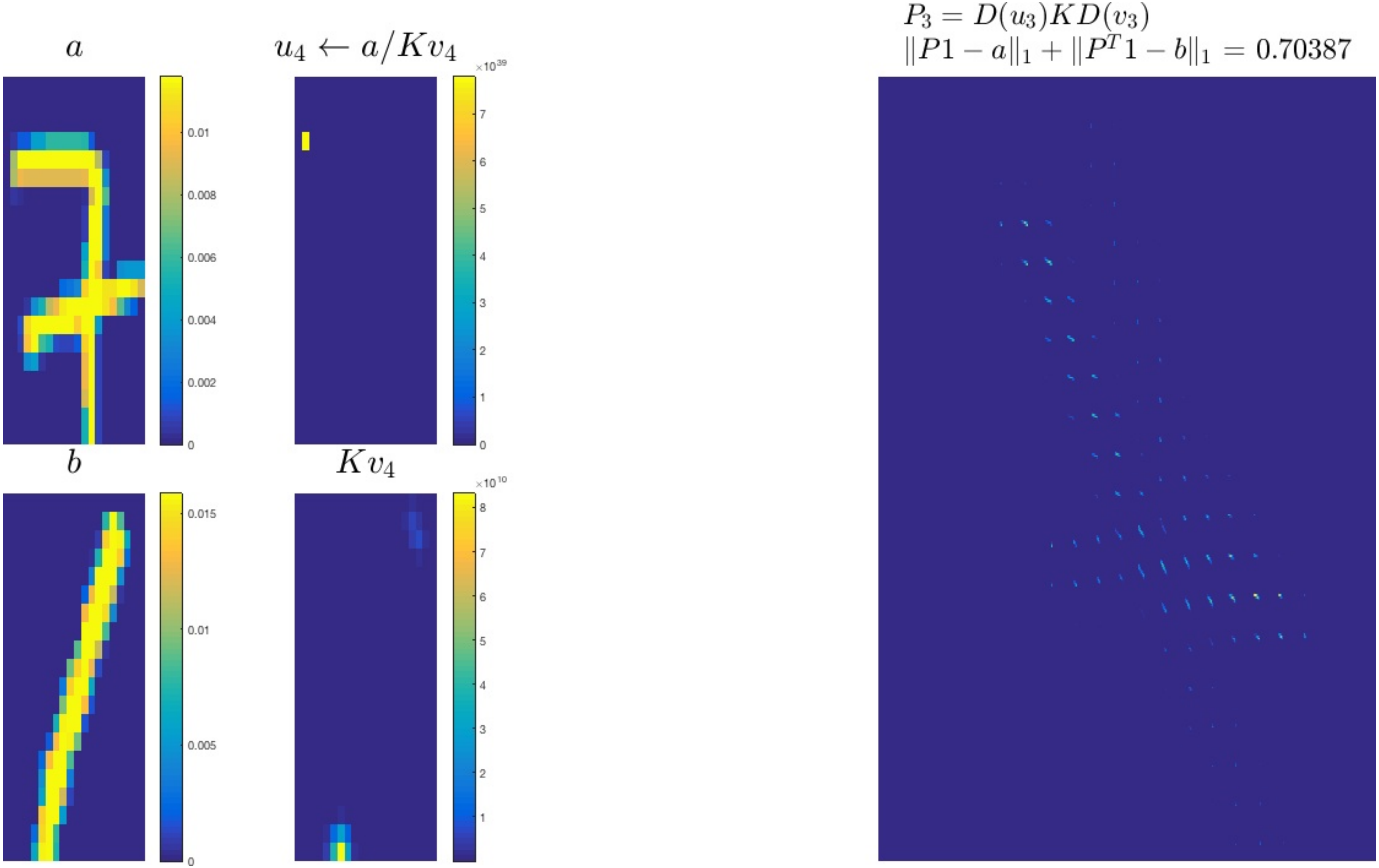


$P_3 = D(u_3)KD(v_3)$

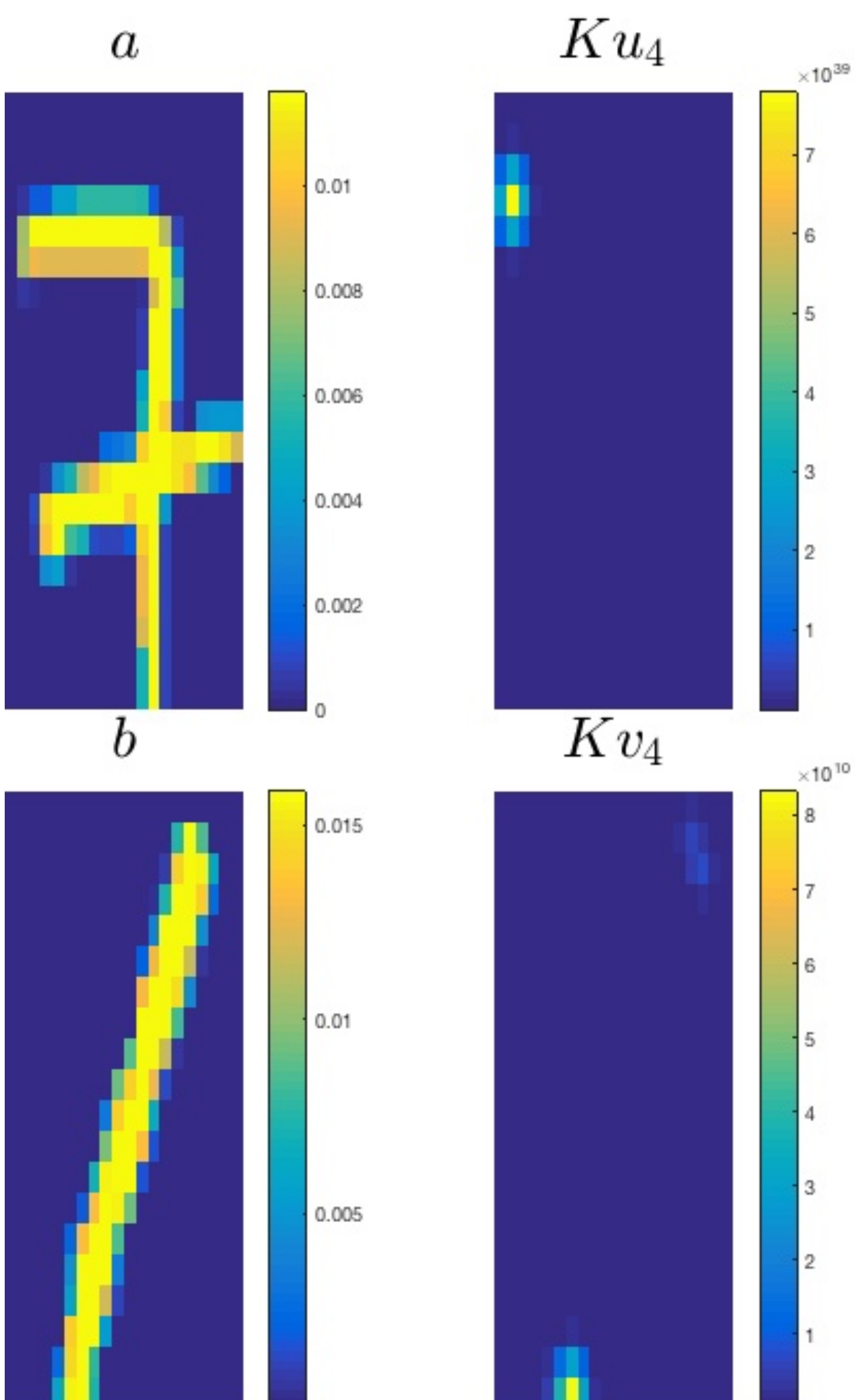
$\|P1 - a\|_1 + \|P^T 1 - b\|_1 = 0.70387$



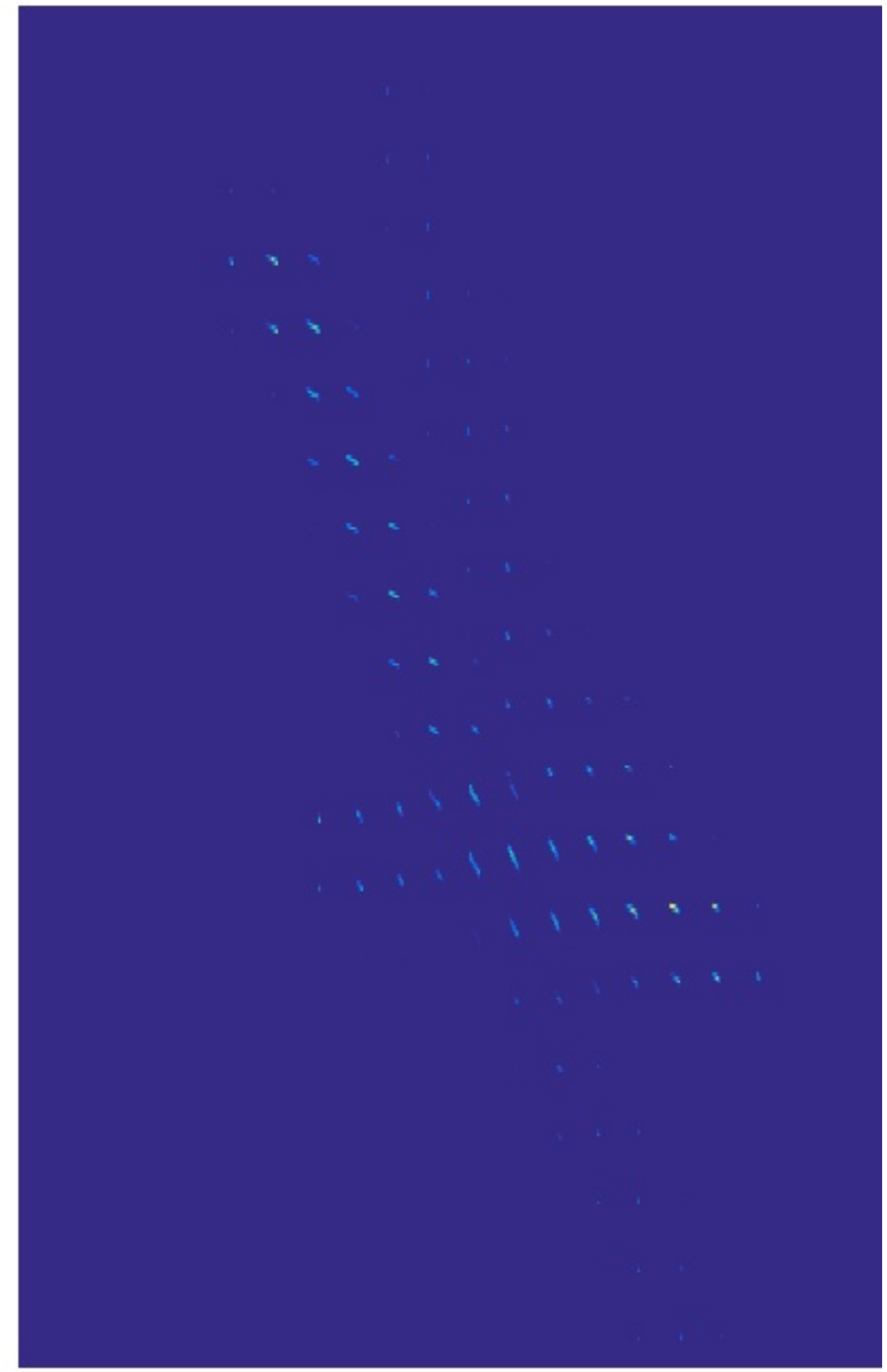
Very Fast EMD Approx. Solver



Very Fast EMD Approx. Solver



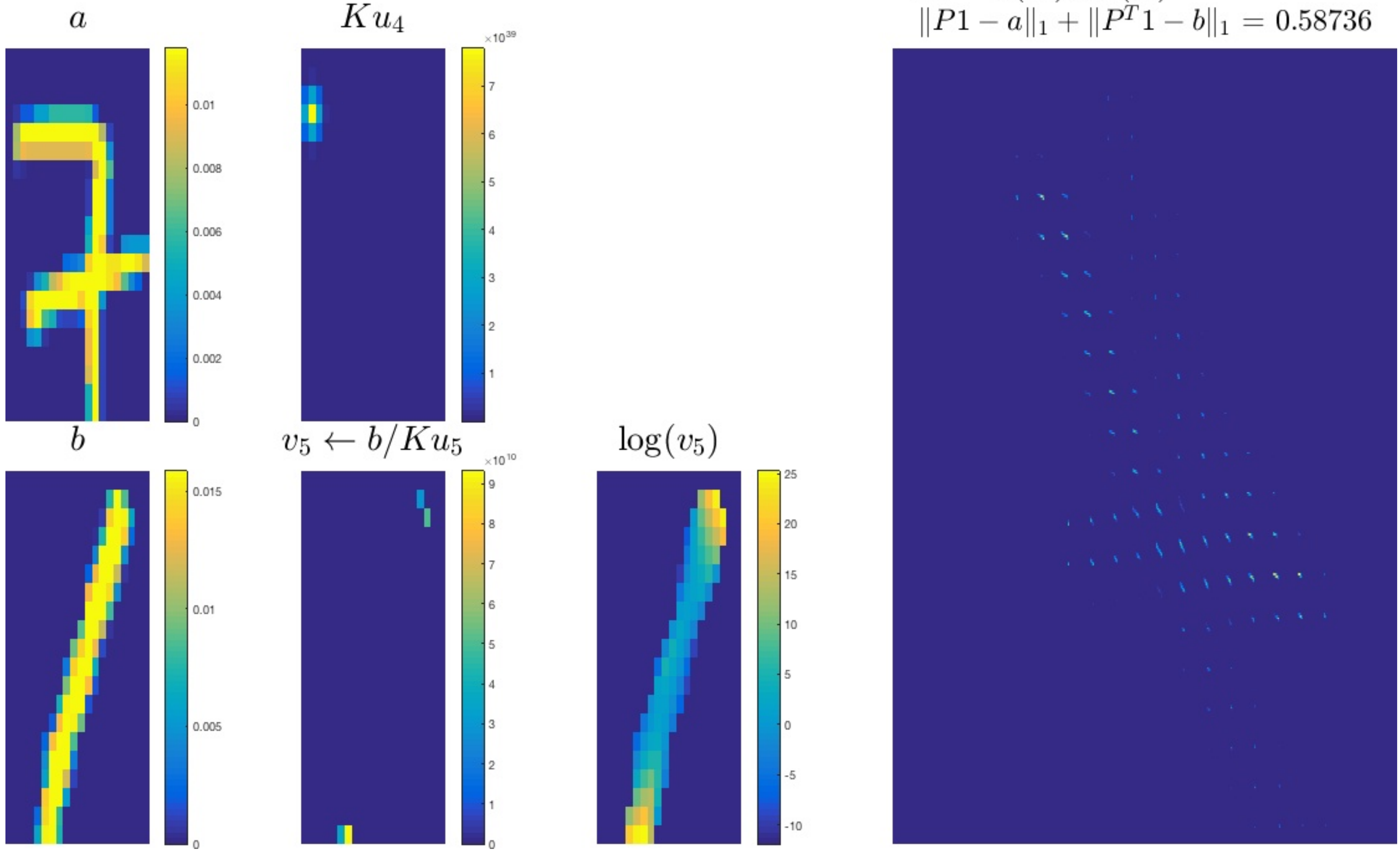
$P_3 = D(u_3)KD(v_3)$
$\|P\mathbb{1} - a\|_1 + \|P^T\mathbb{1} - b\|_1 = 0.70387$



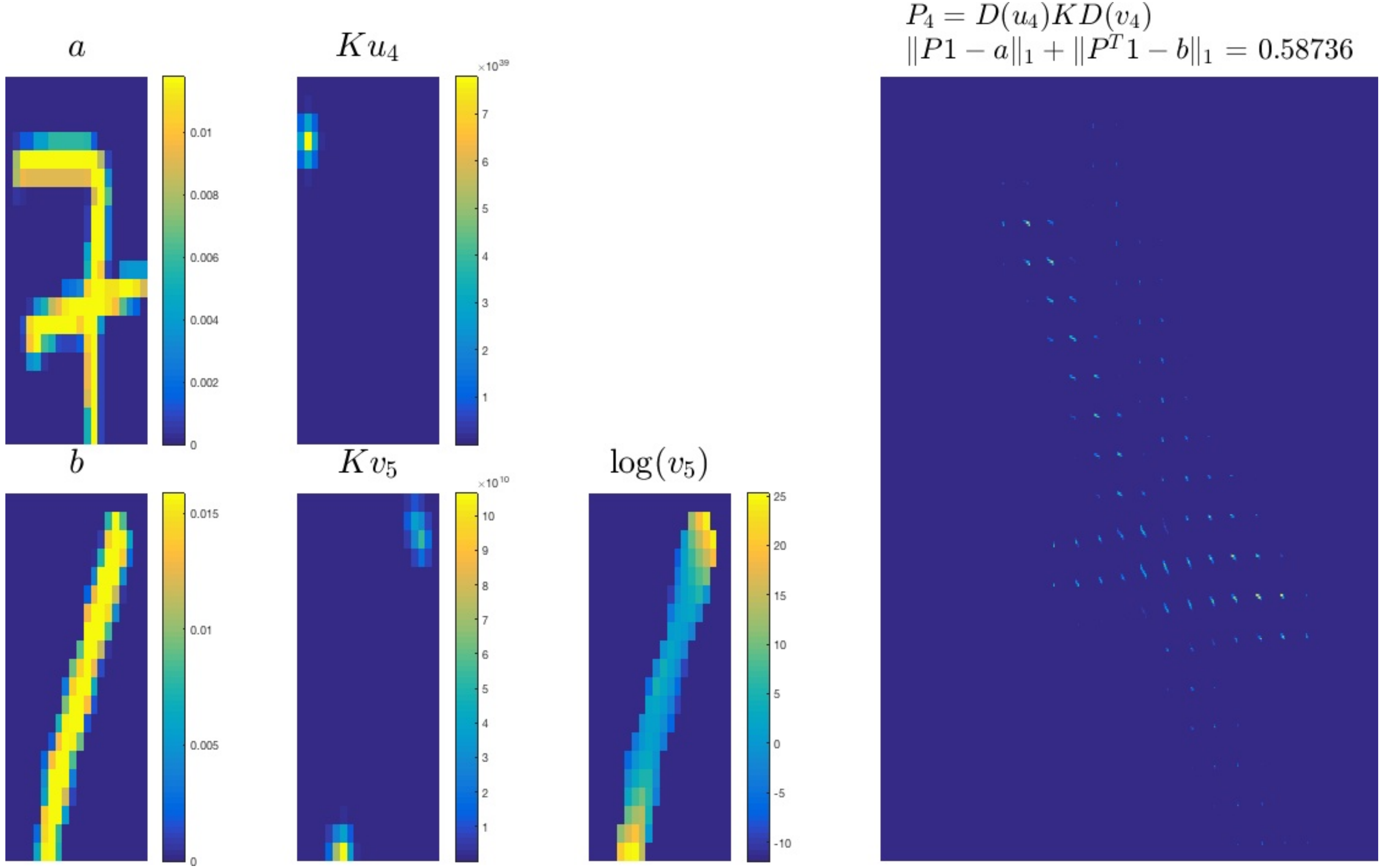
Very Fast EMD Approx. Solver

$P_4 = D(u_4)KD(v_4)$

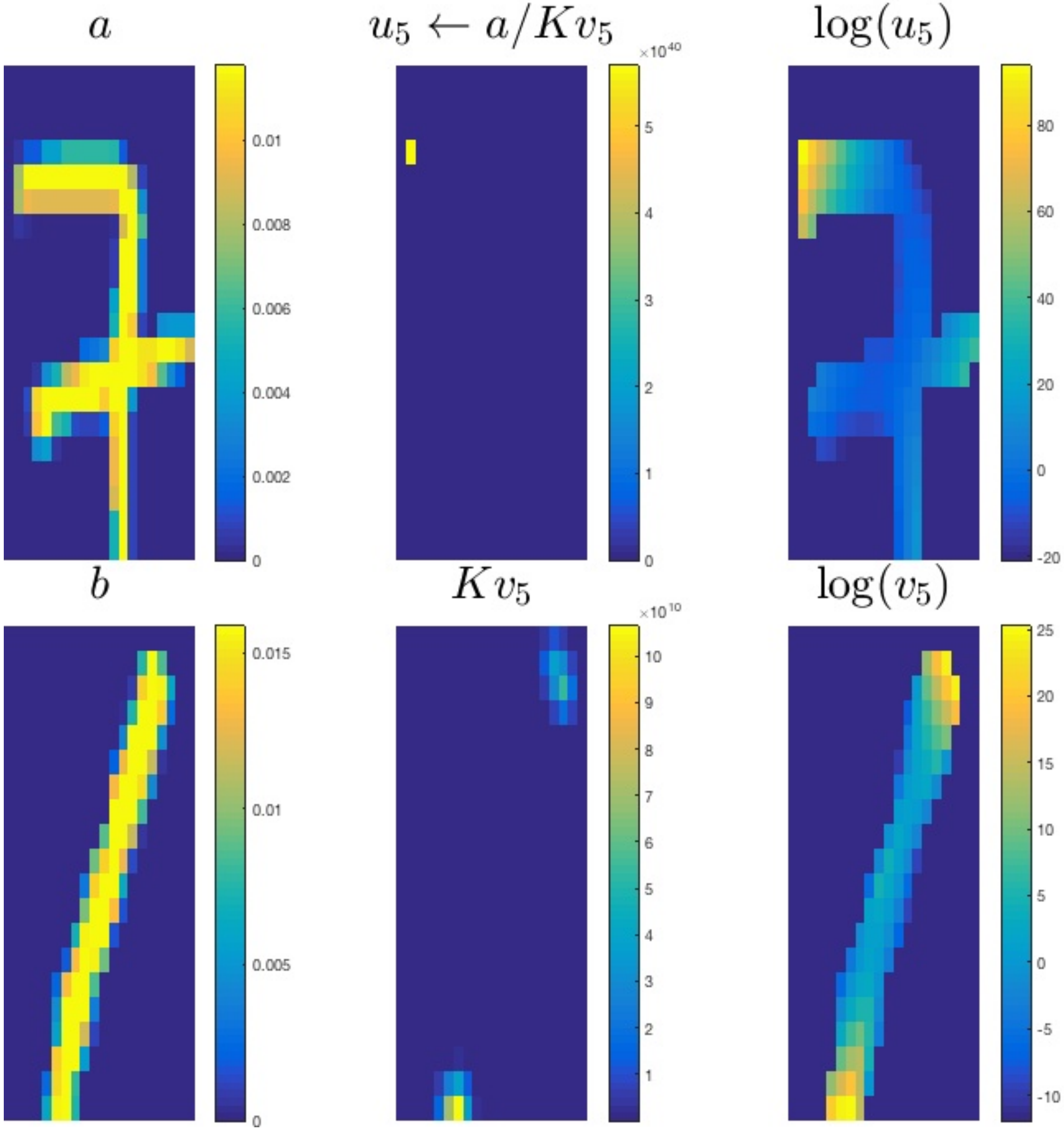
$\|P1 - a\|_1 + \|P^T1 - b\|_1 = 0.58736$



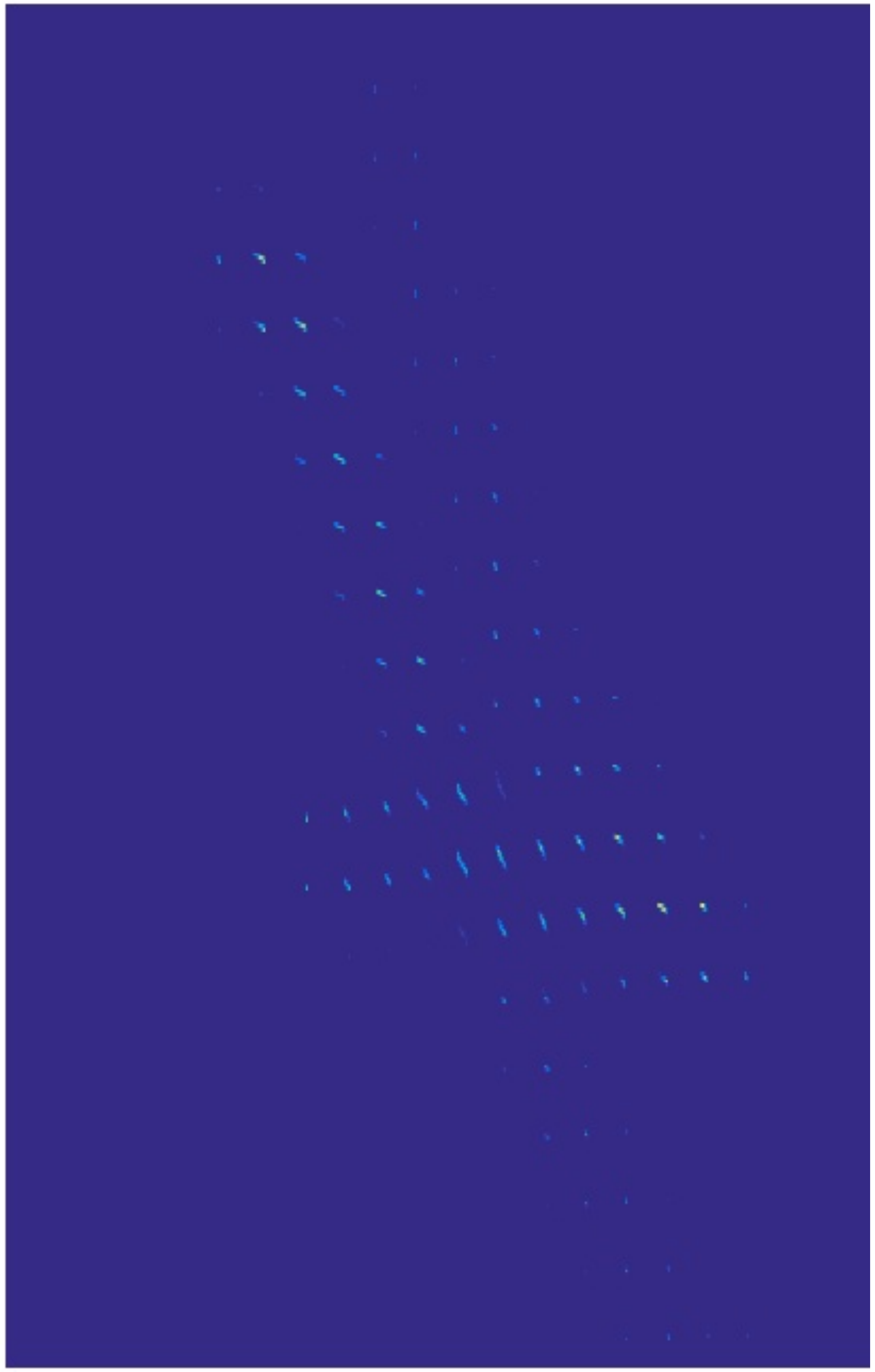
Very Fast EMD Approx. Solver



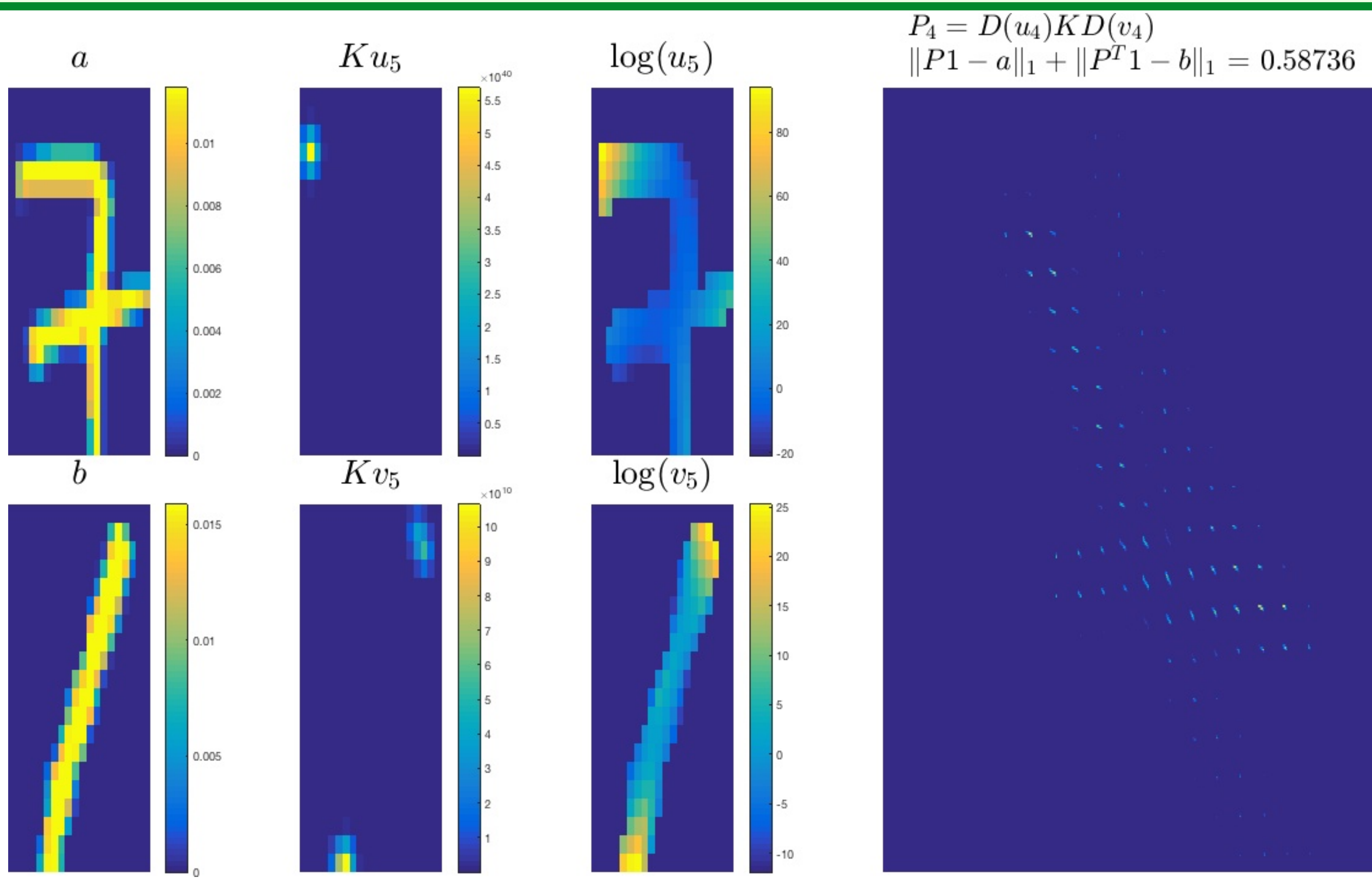
Very Fast EMD Approx. Solver



$P_4 = D(u_4)KD(v_4)$
$\|P\mathbb{1} - a\|_1 + \|P^T\mathbb{1} - b\|_1 = 0.58736$



Very Fast EMD Approx. Solver



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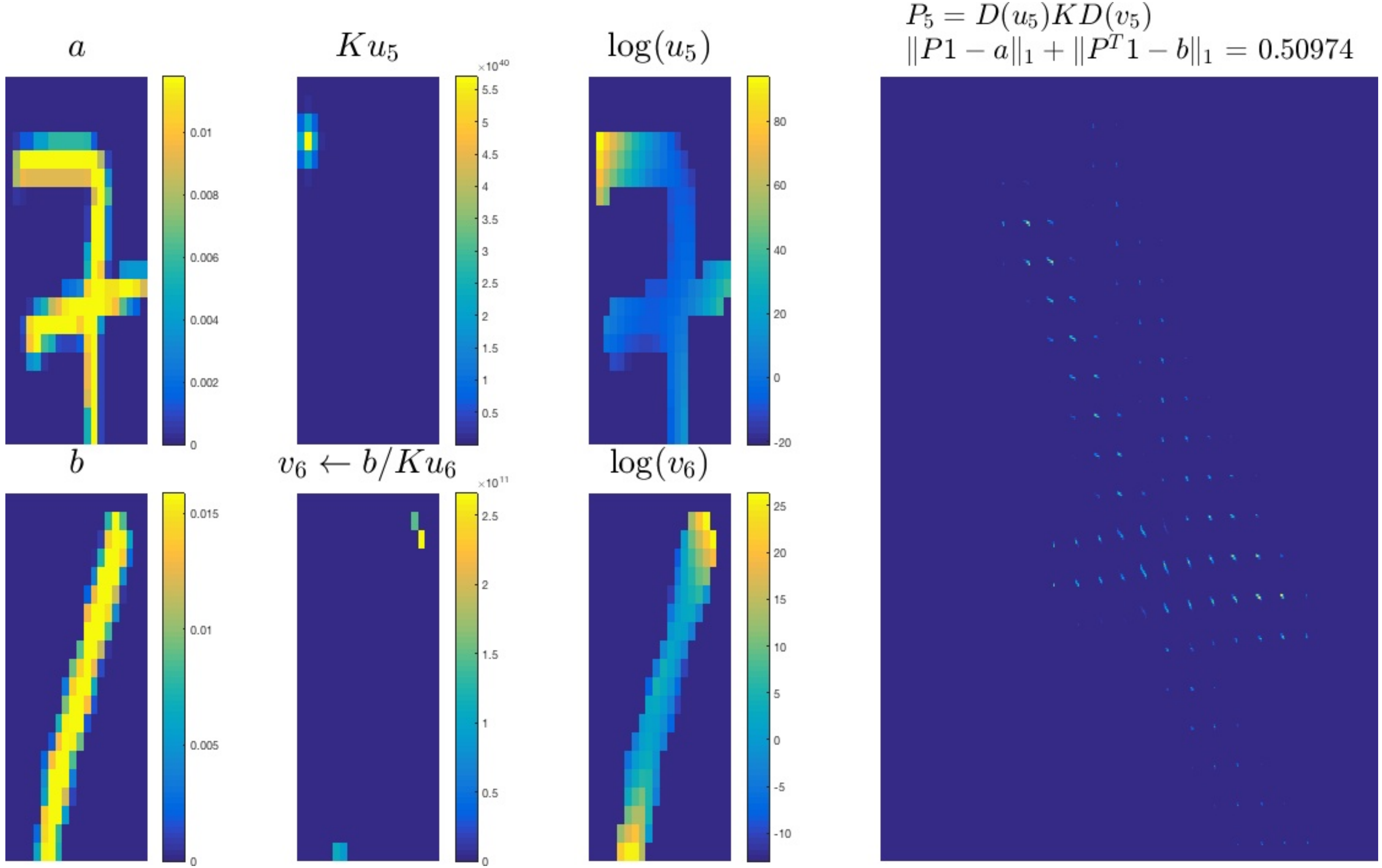
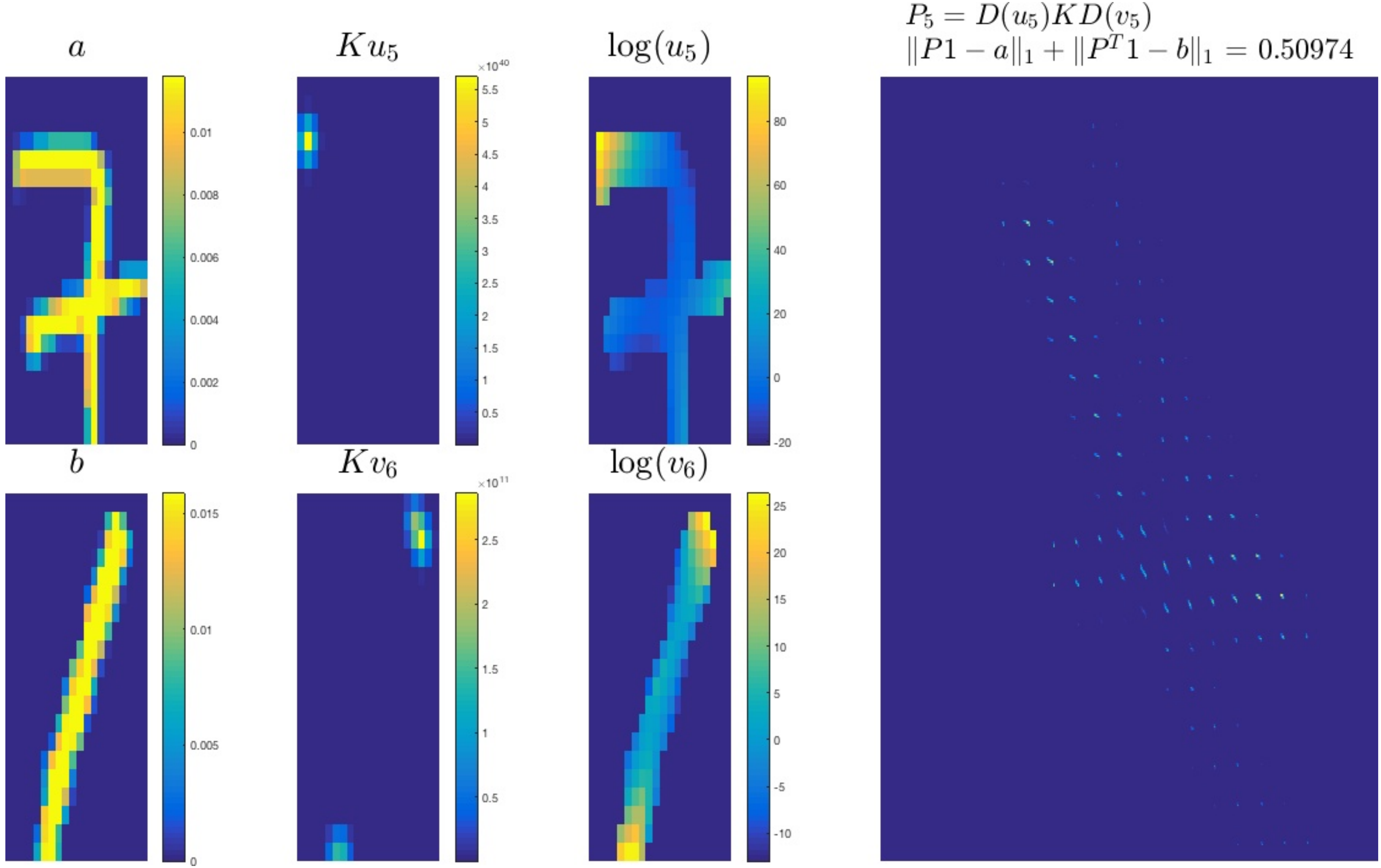
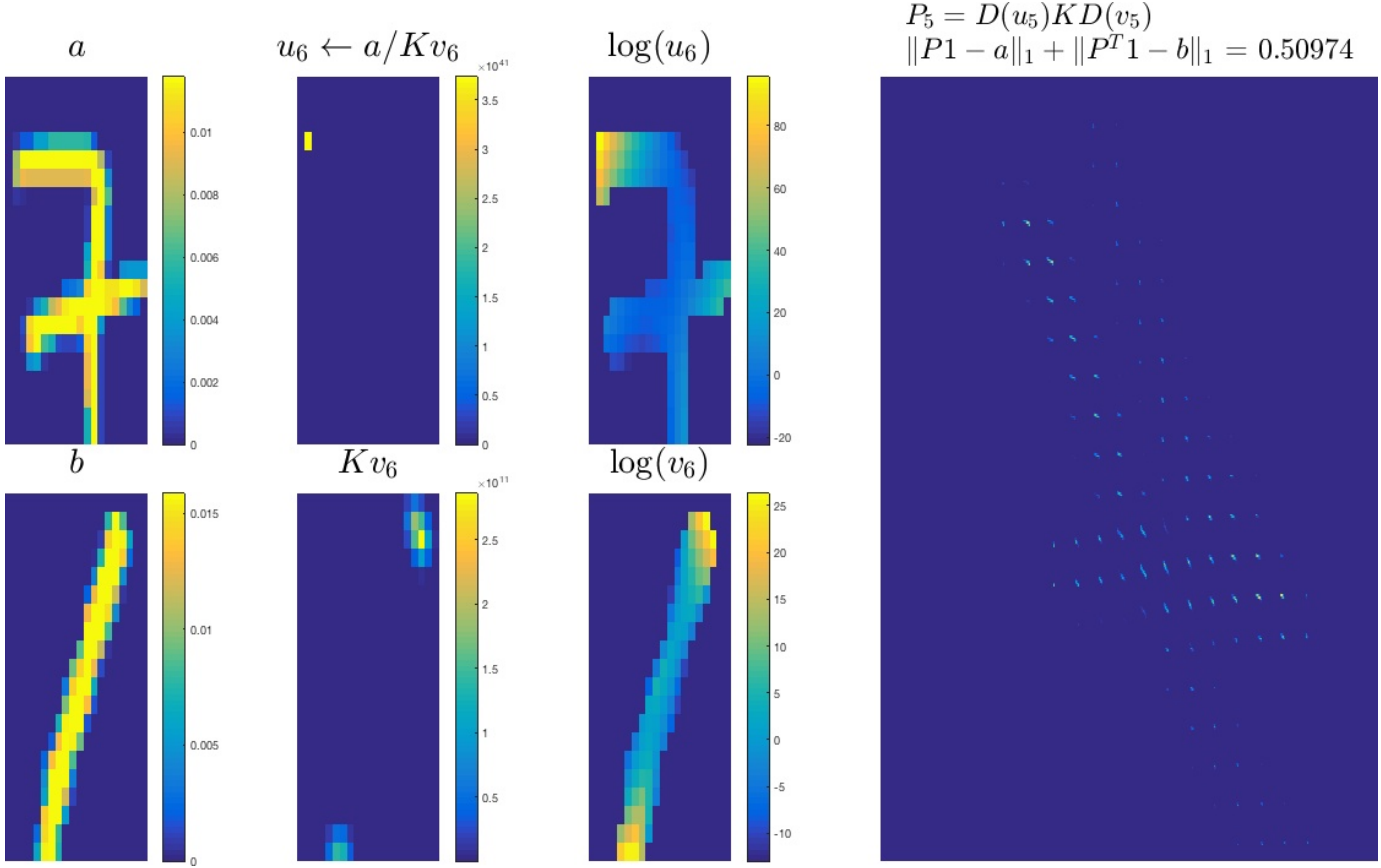


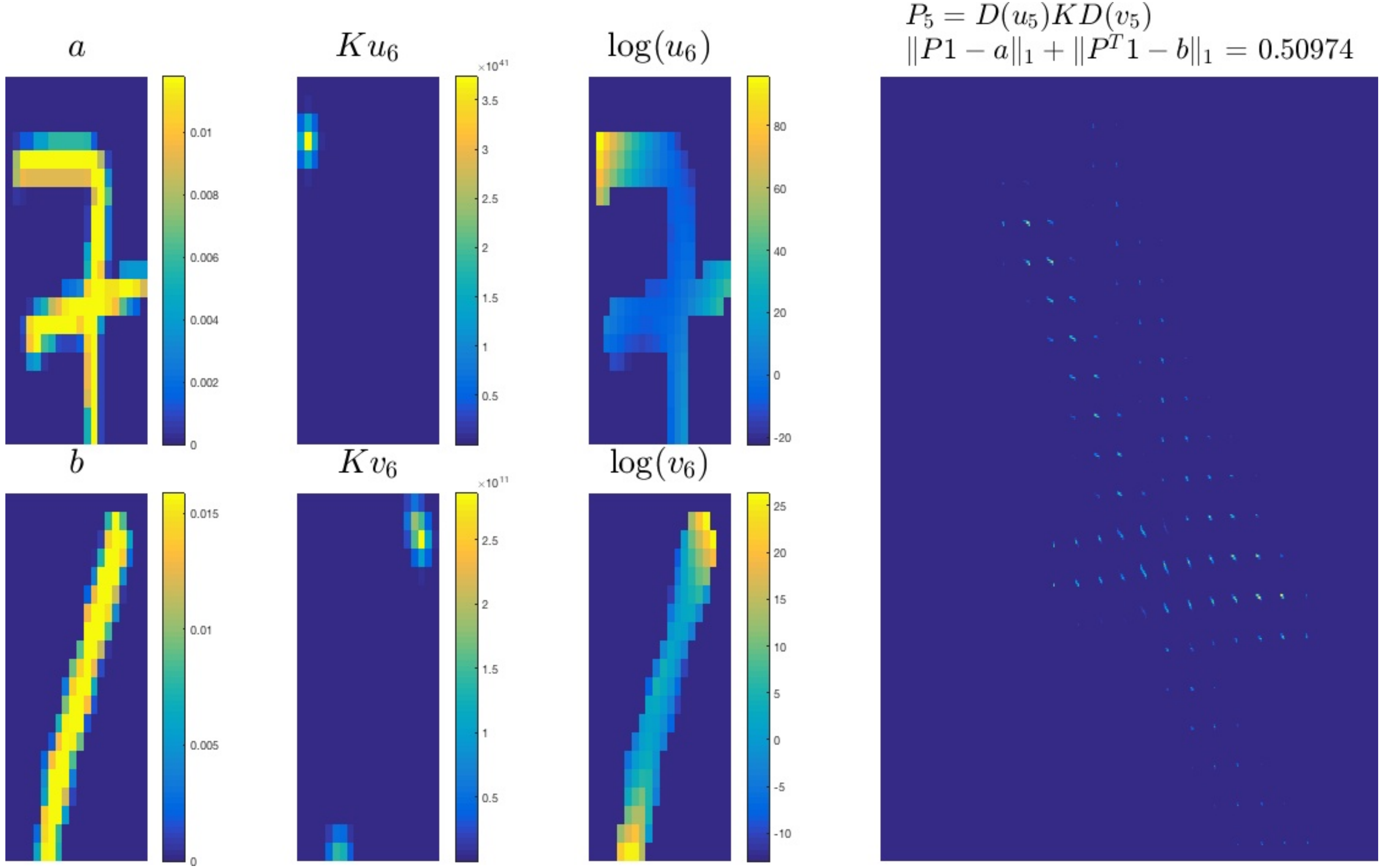
Very Fast EMD Approx. Solver



Very Fast EMD Approx. Solver



Very Fast EMD Approx. Solver



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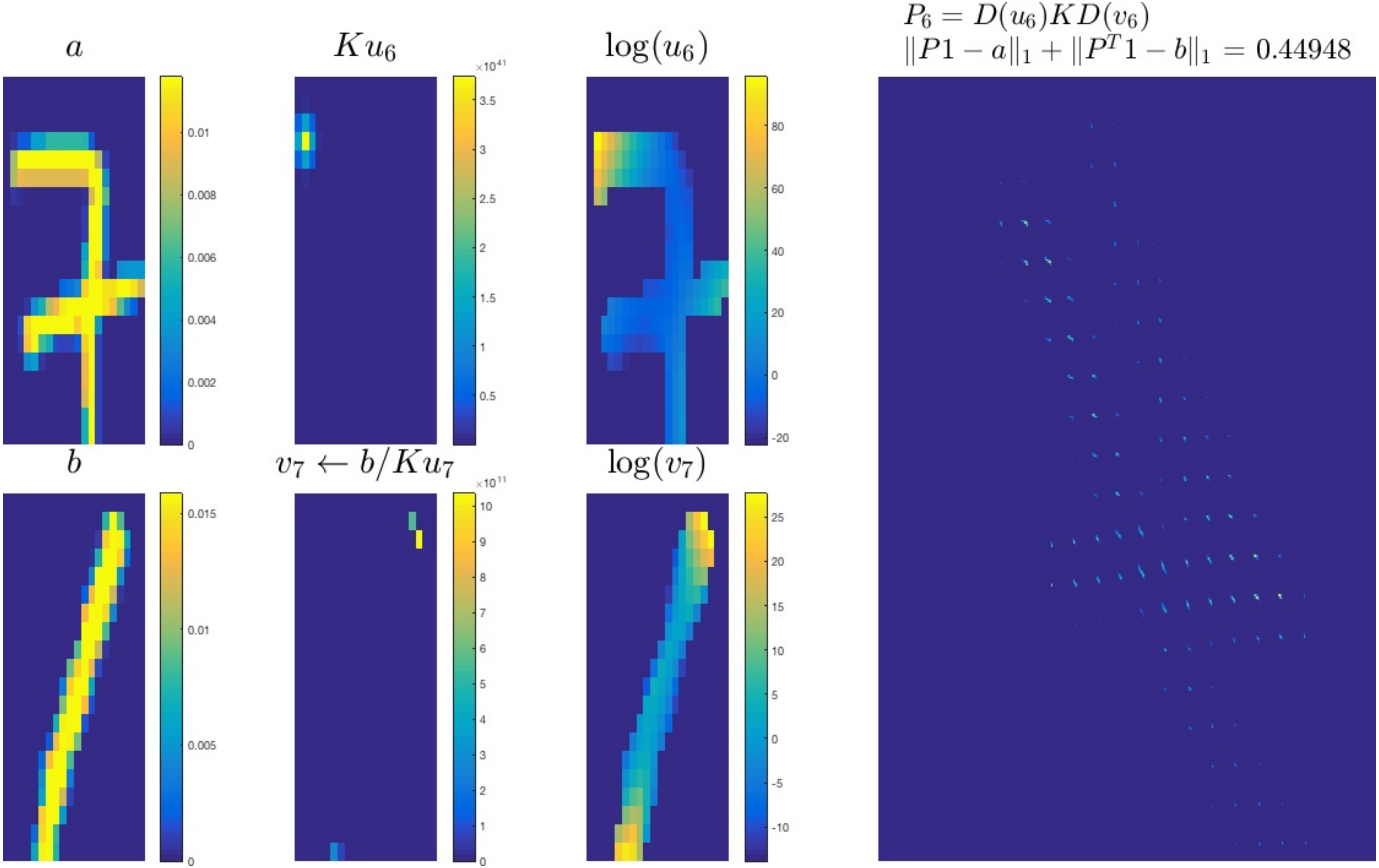
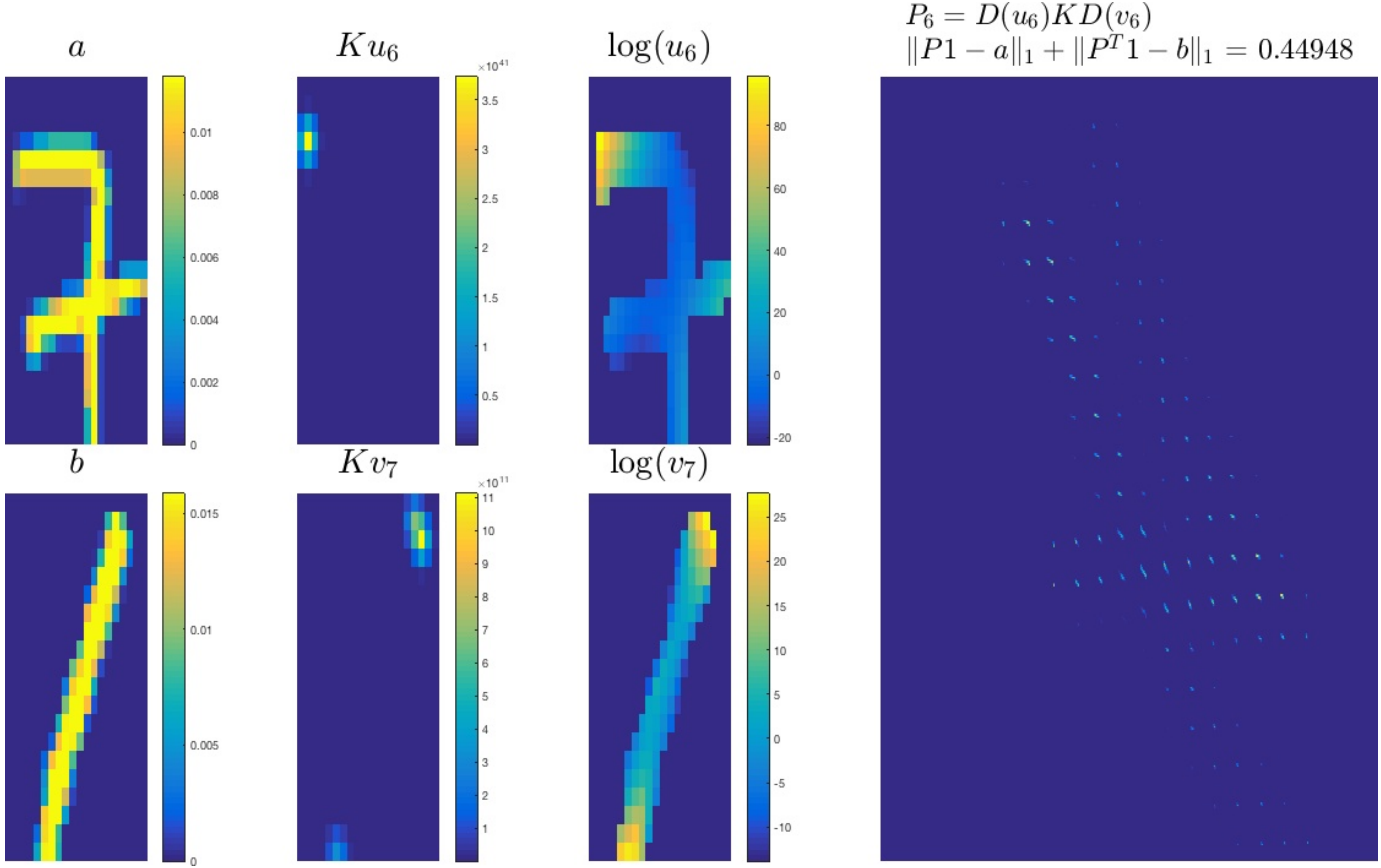


Very Fast EMD Approx. Solver



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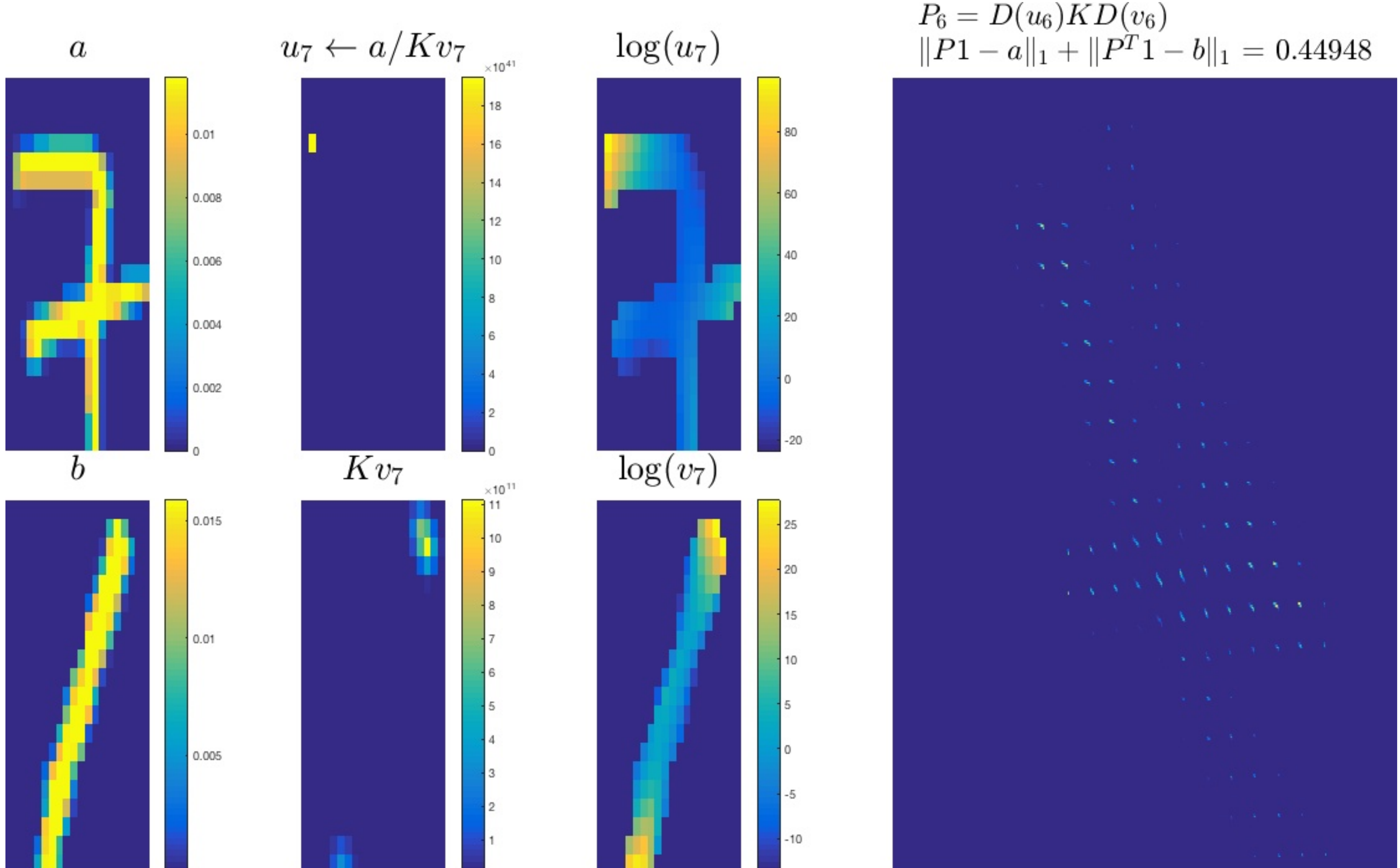

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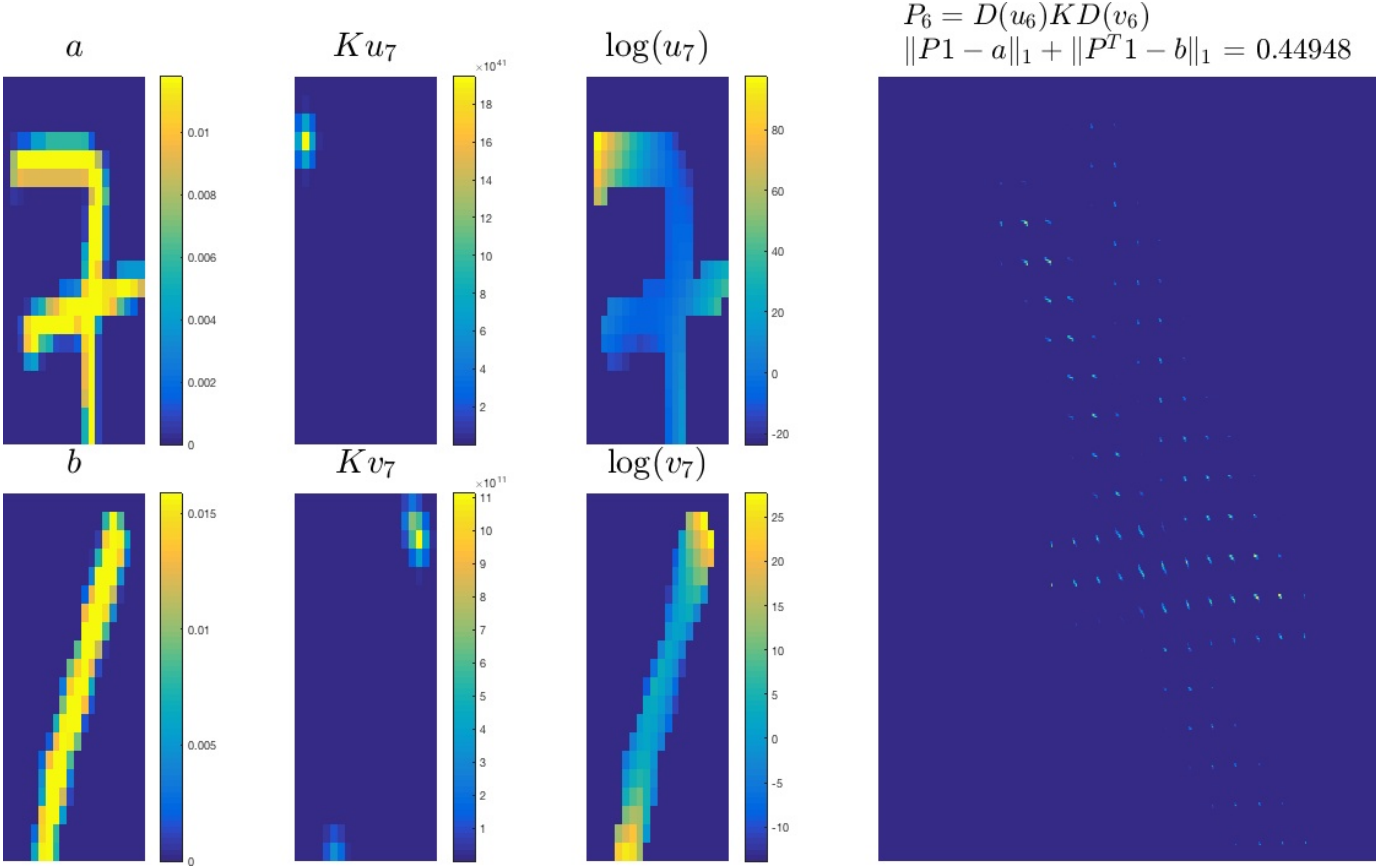

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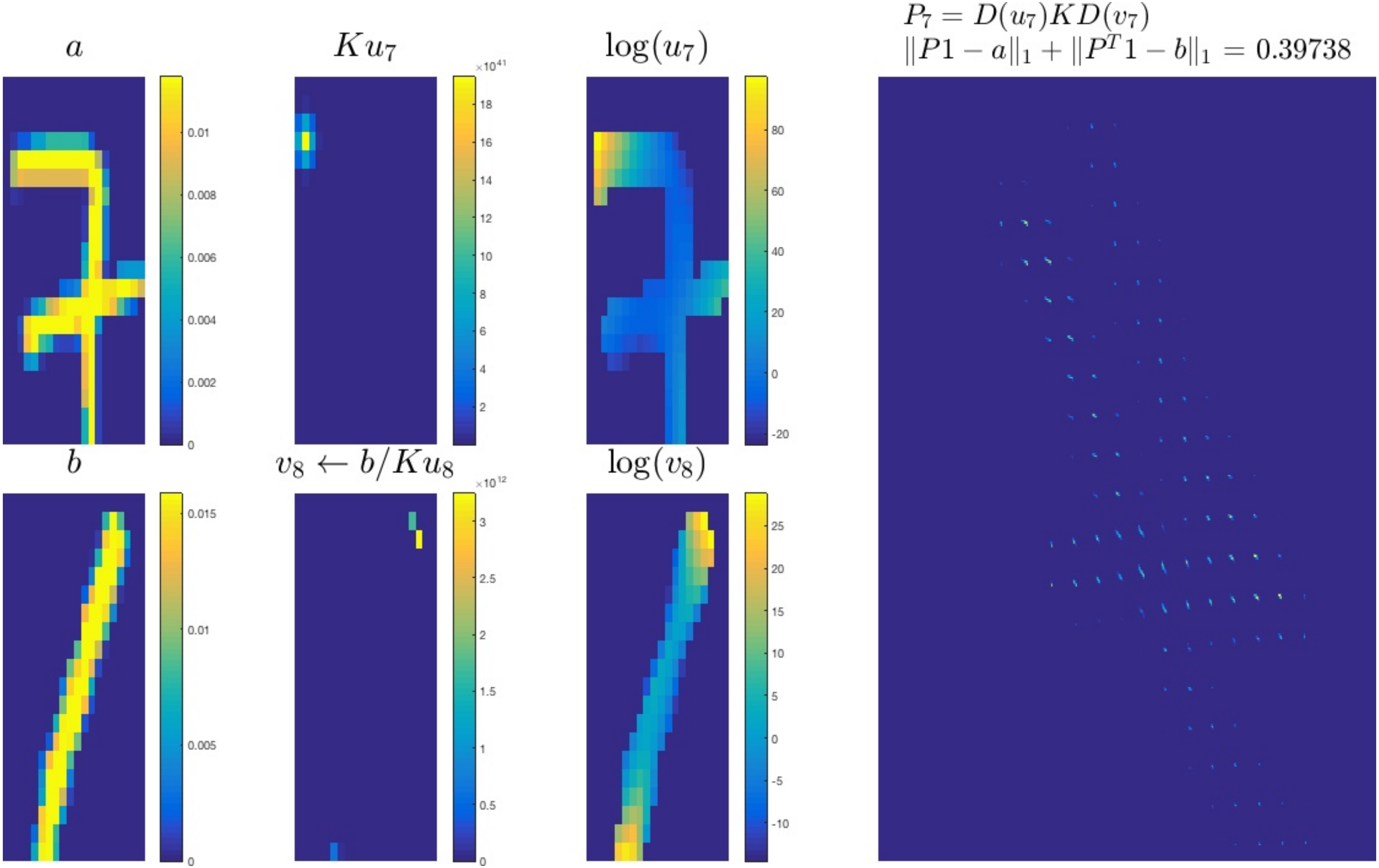
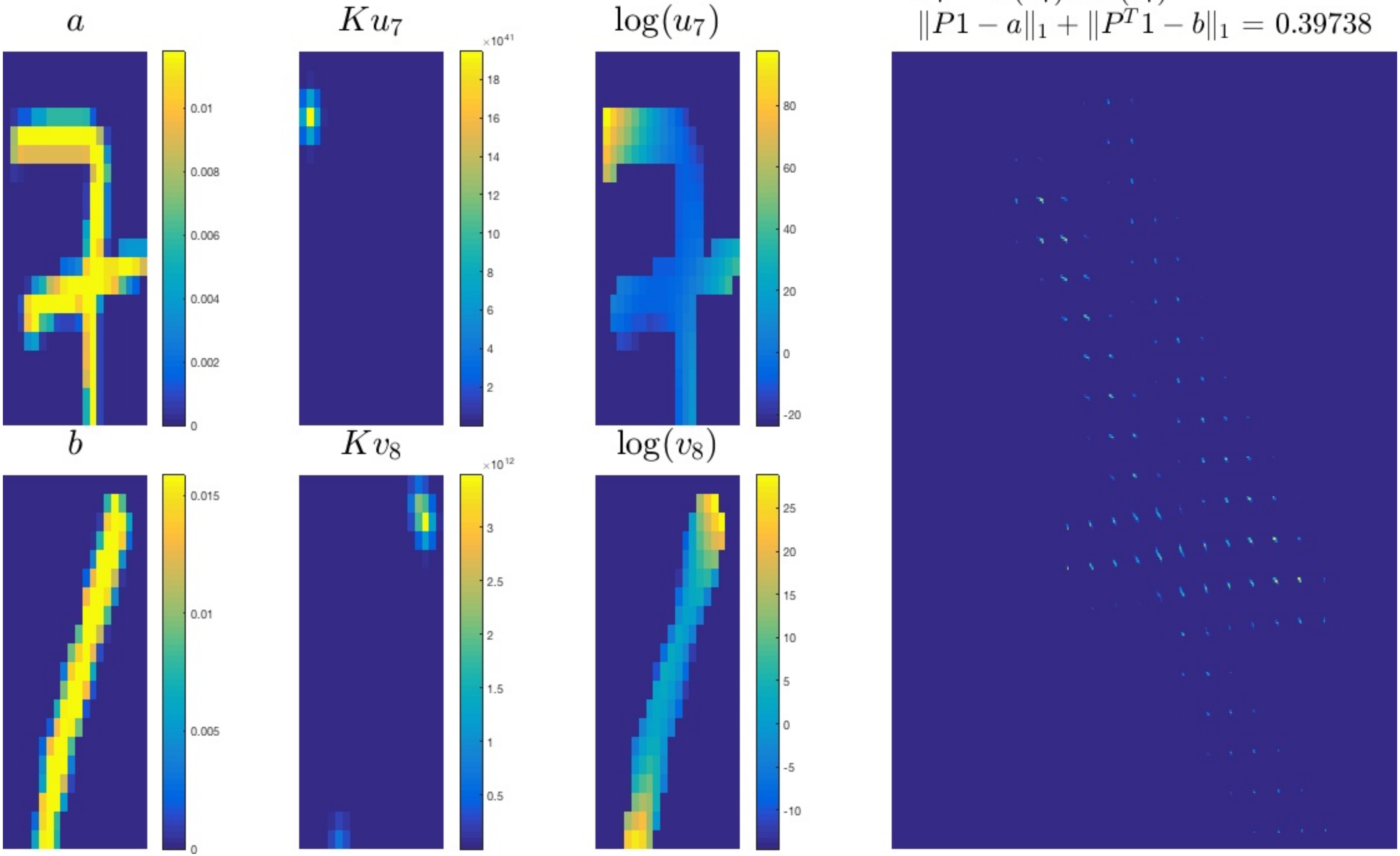


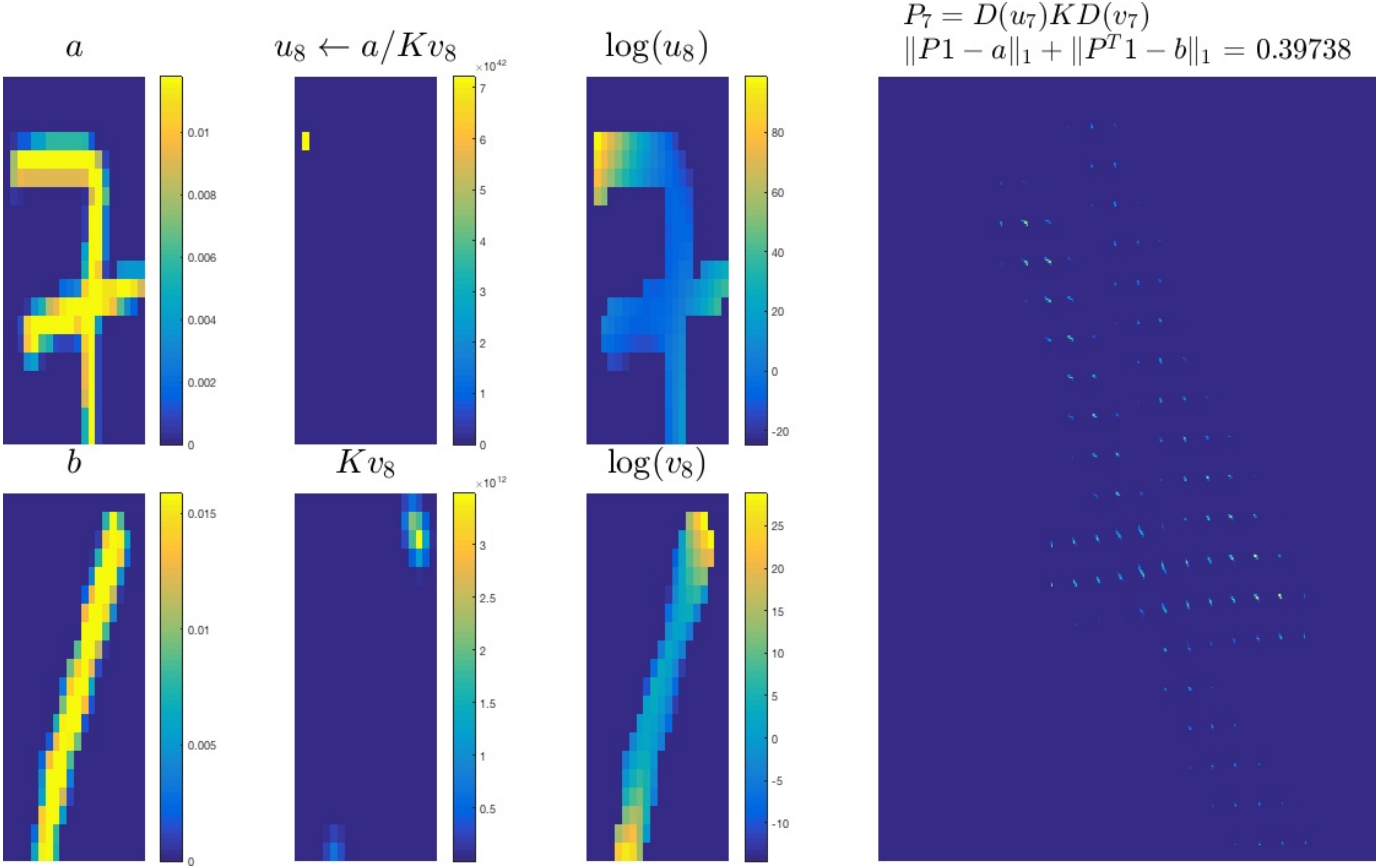
Very Fast EMD Approx. Solver

$P_7 = D(u_7)KD(v_7)$

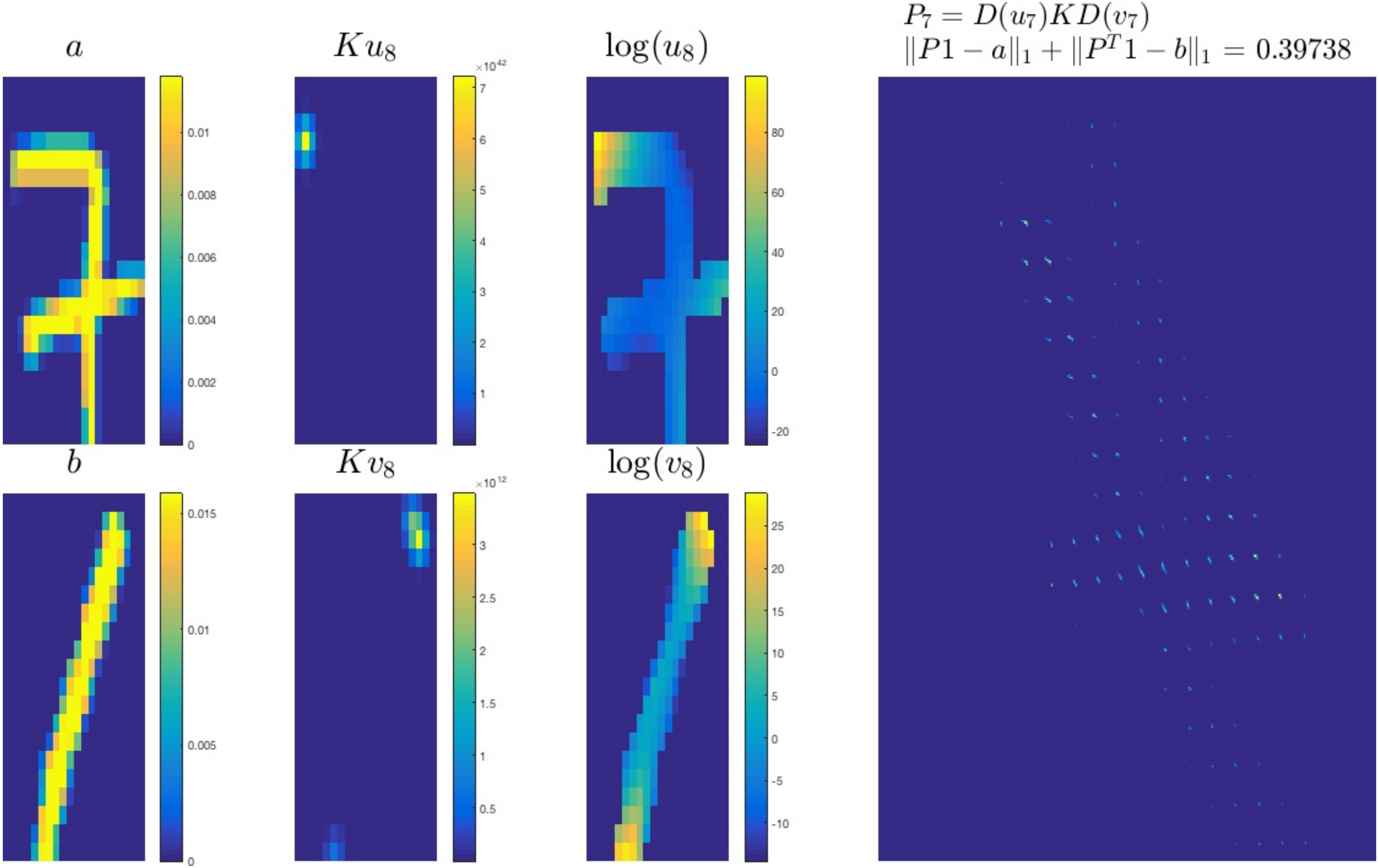
$\|P1 - a\|_1 + \|P^T 1 - b\|_1 = 0.39738$



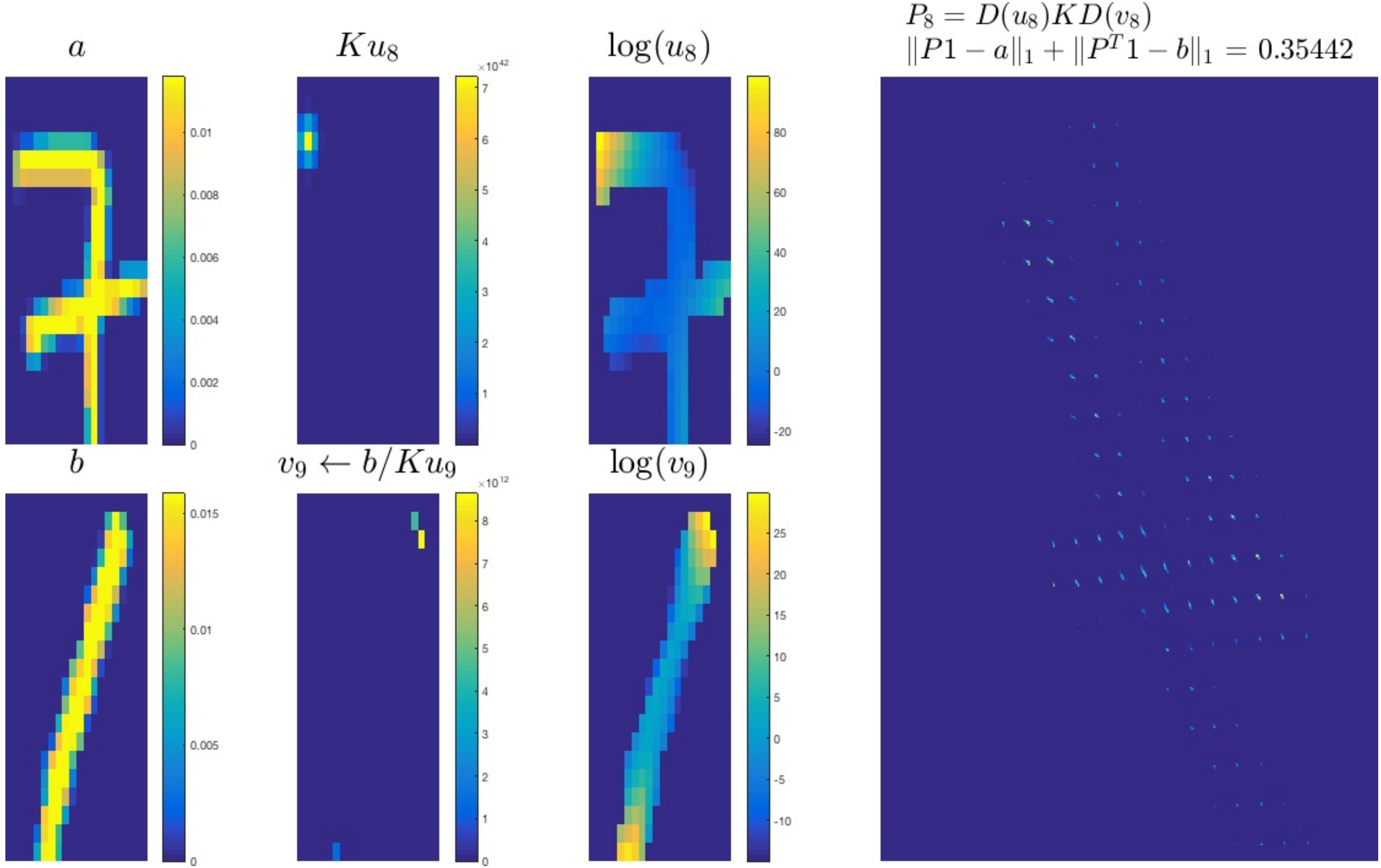
Very Fast EMD Approx. Solver



Very Fast EMD Approx. Solver



Very Fast EMD Approx. Solver



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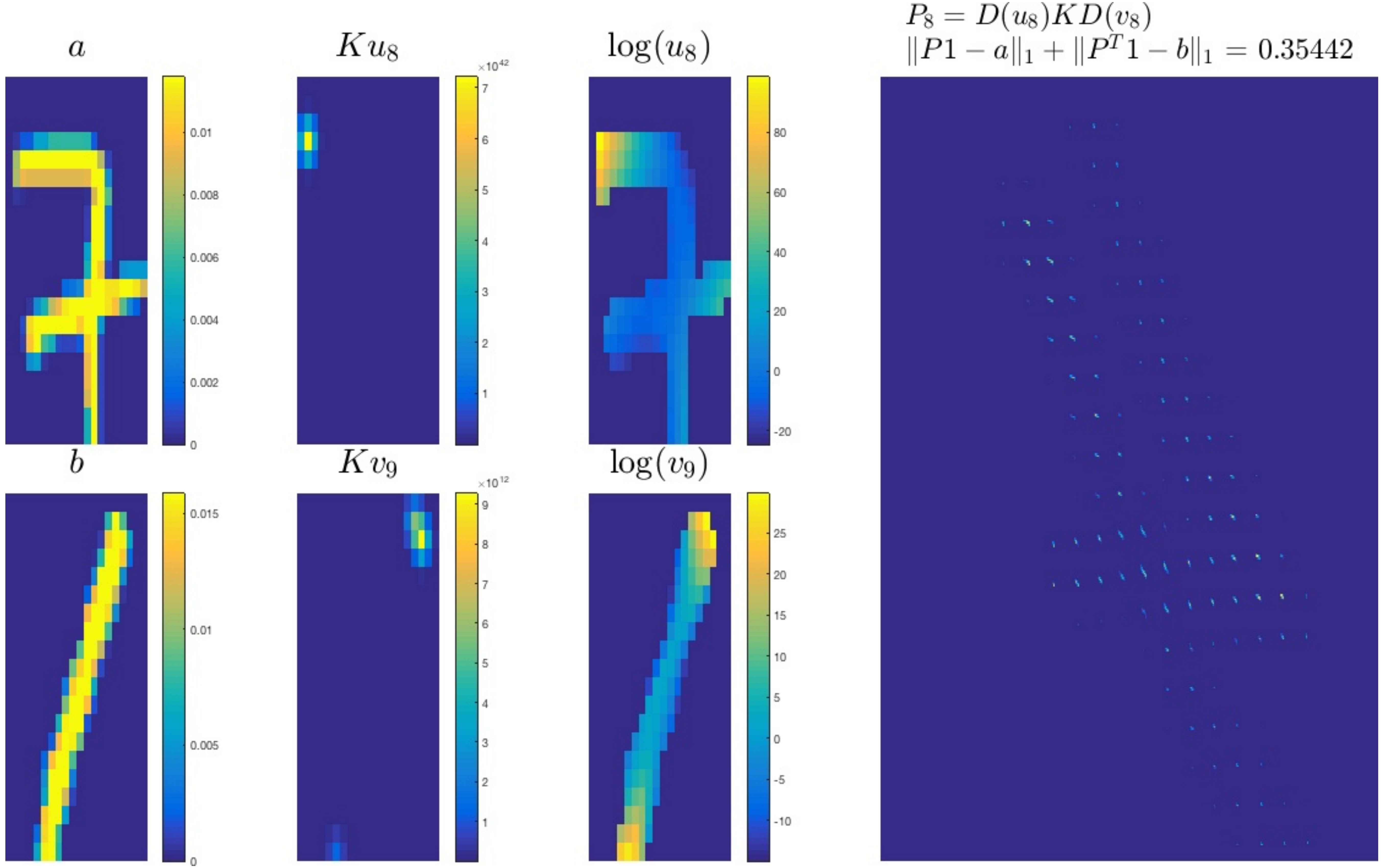
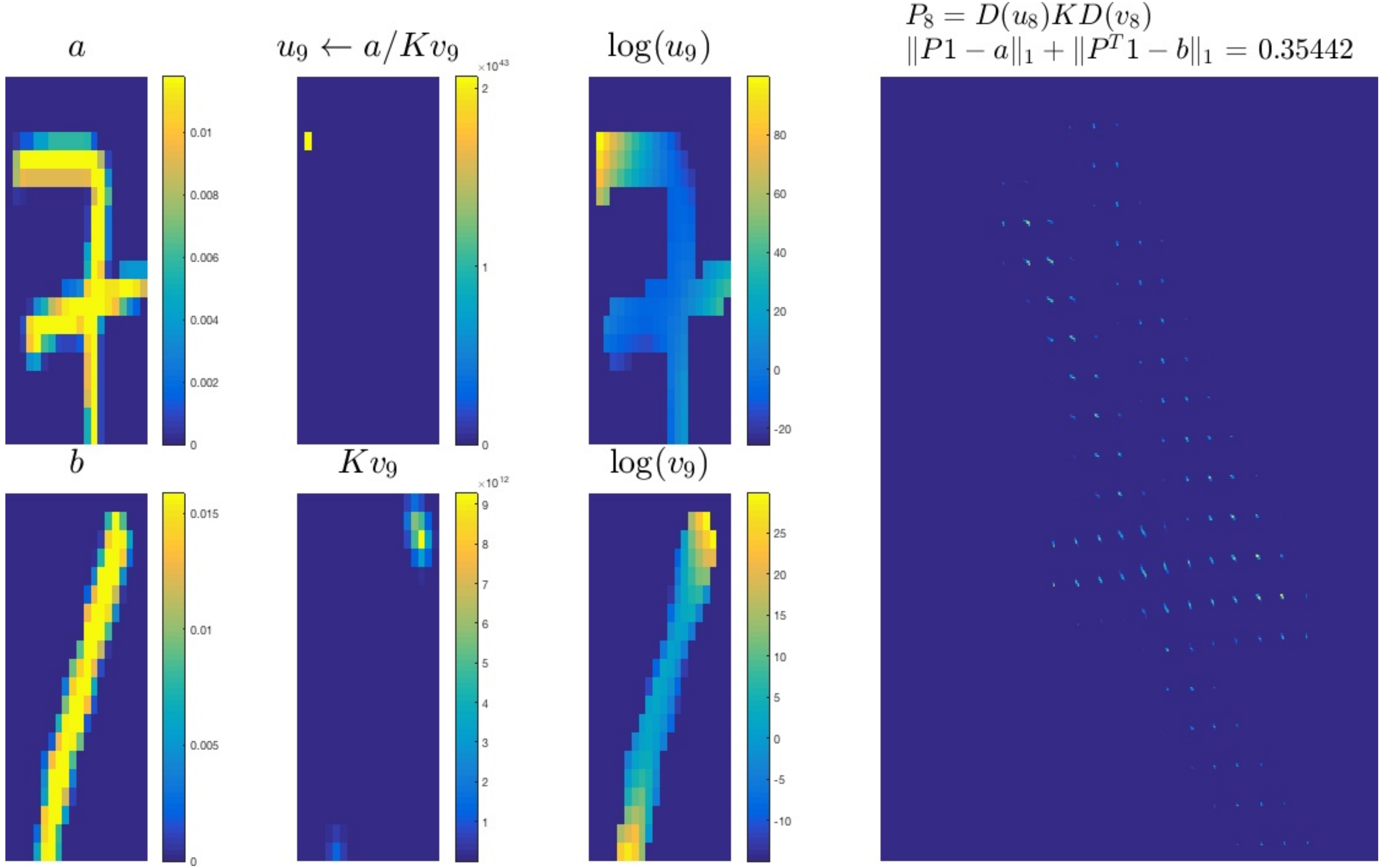


Very Fast EMD Approx. Solver



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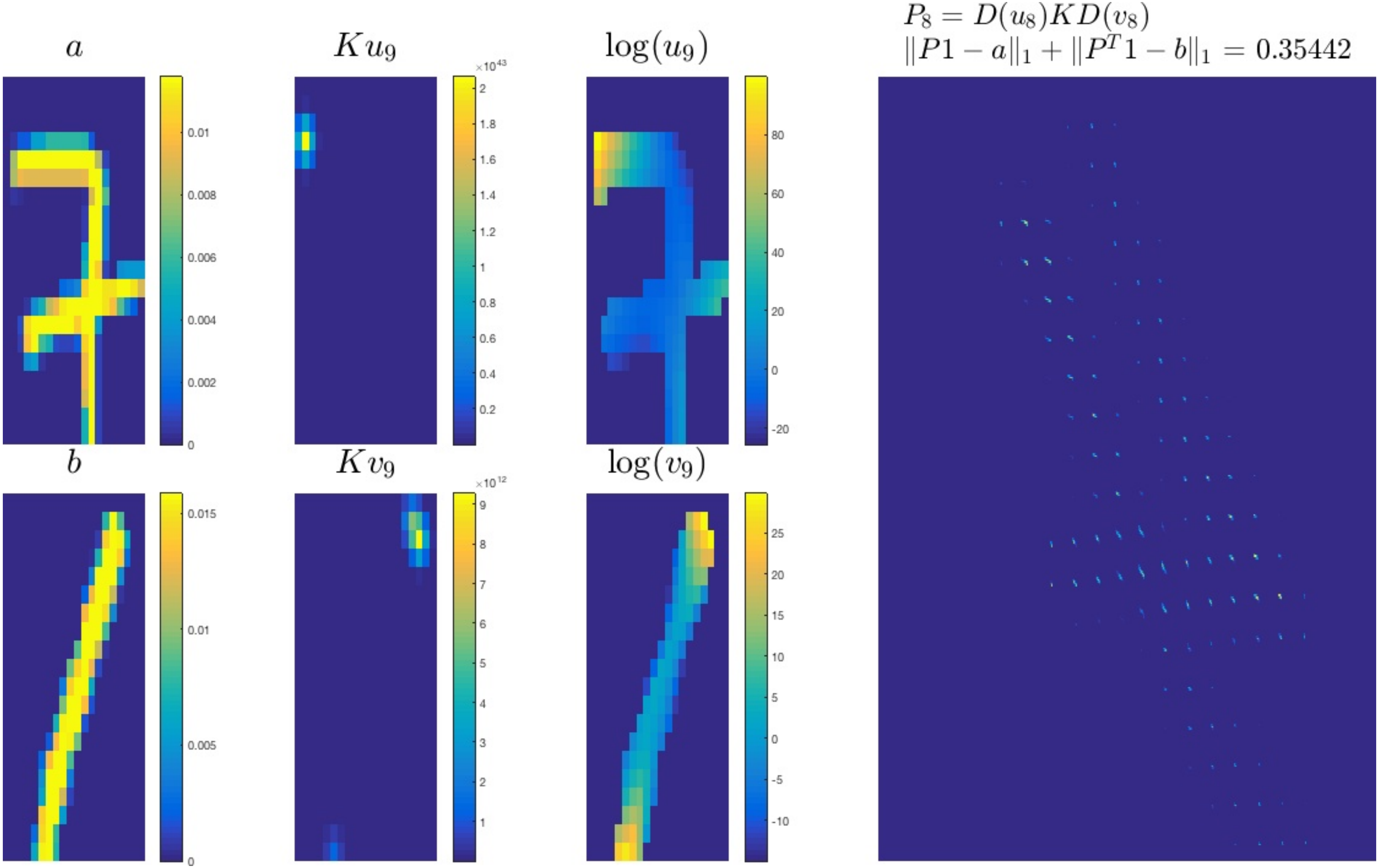
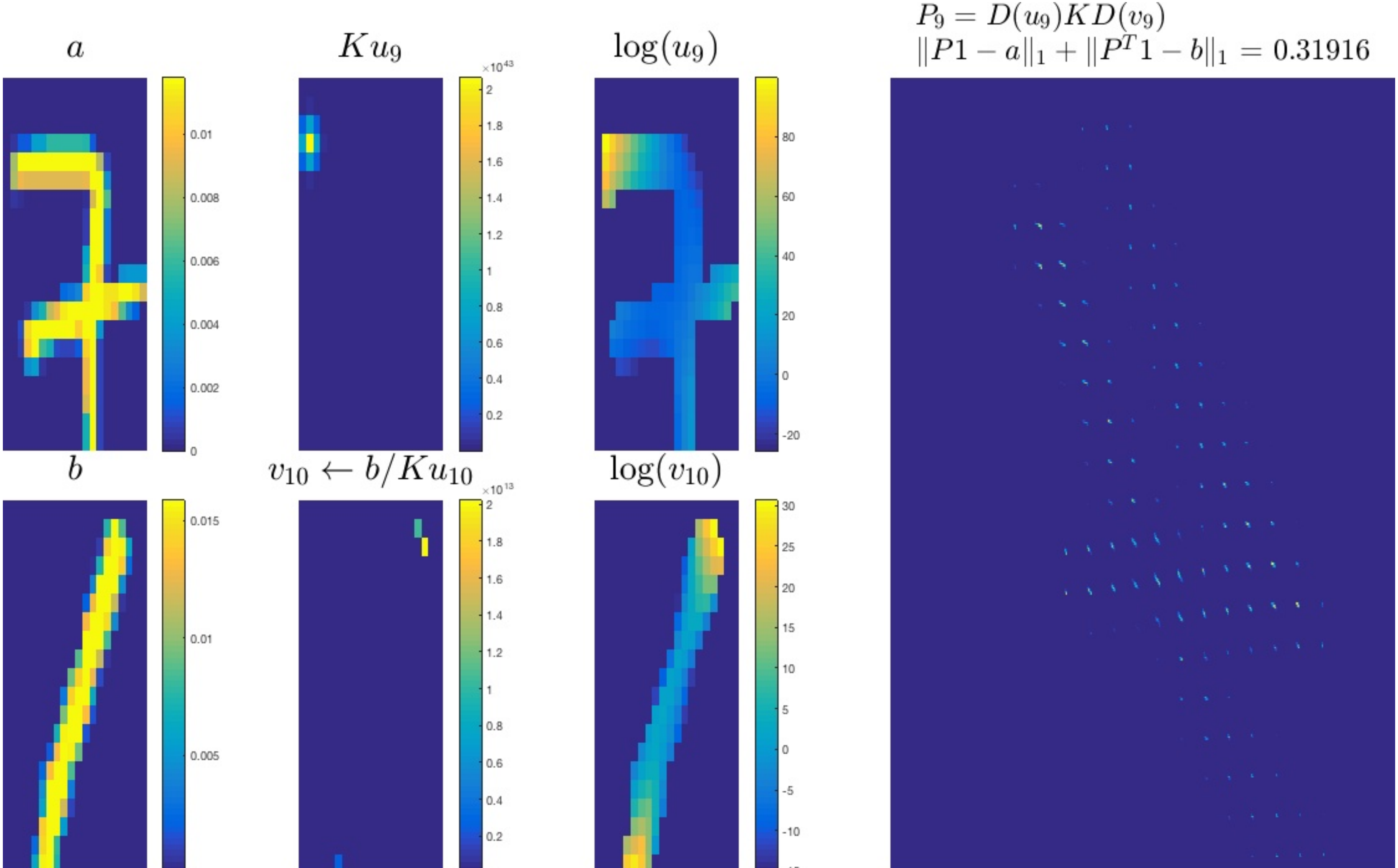


Very Fast EMD Approx. Solver



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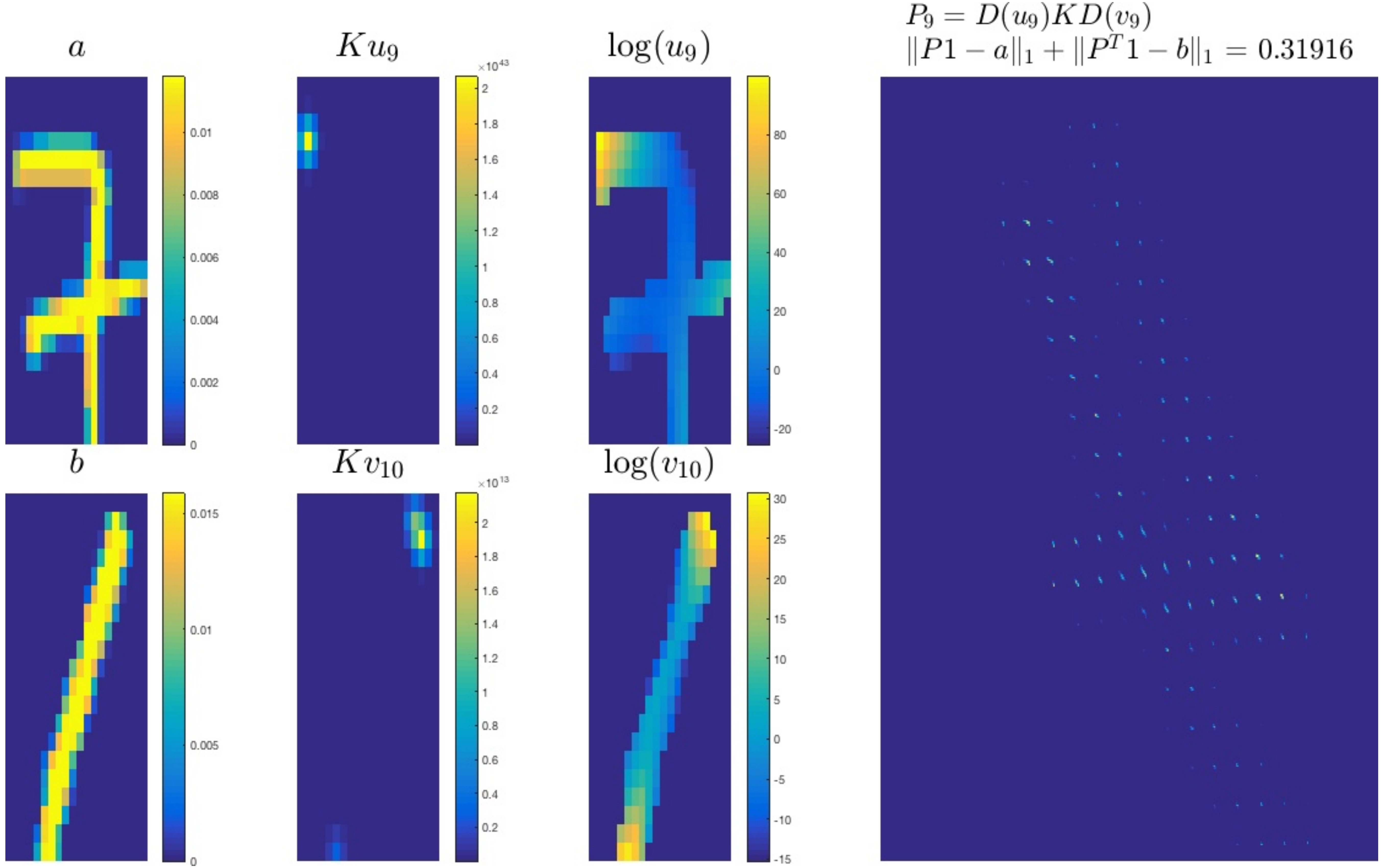

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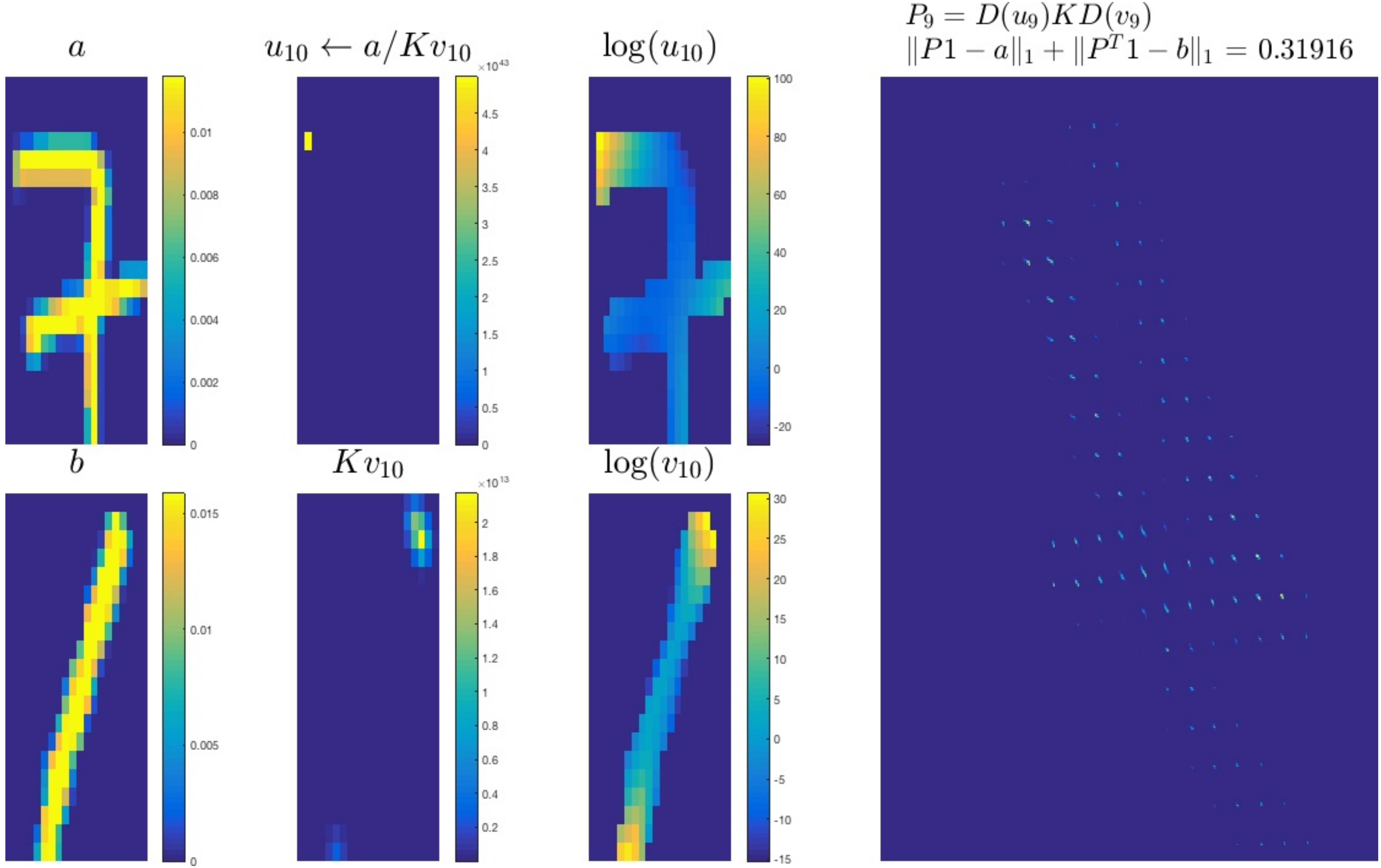
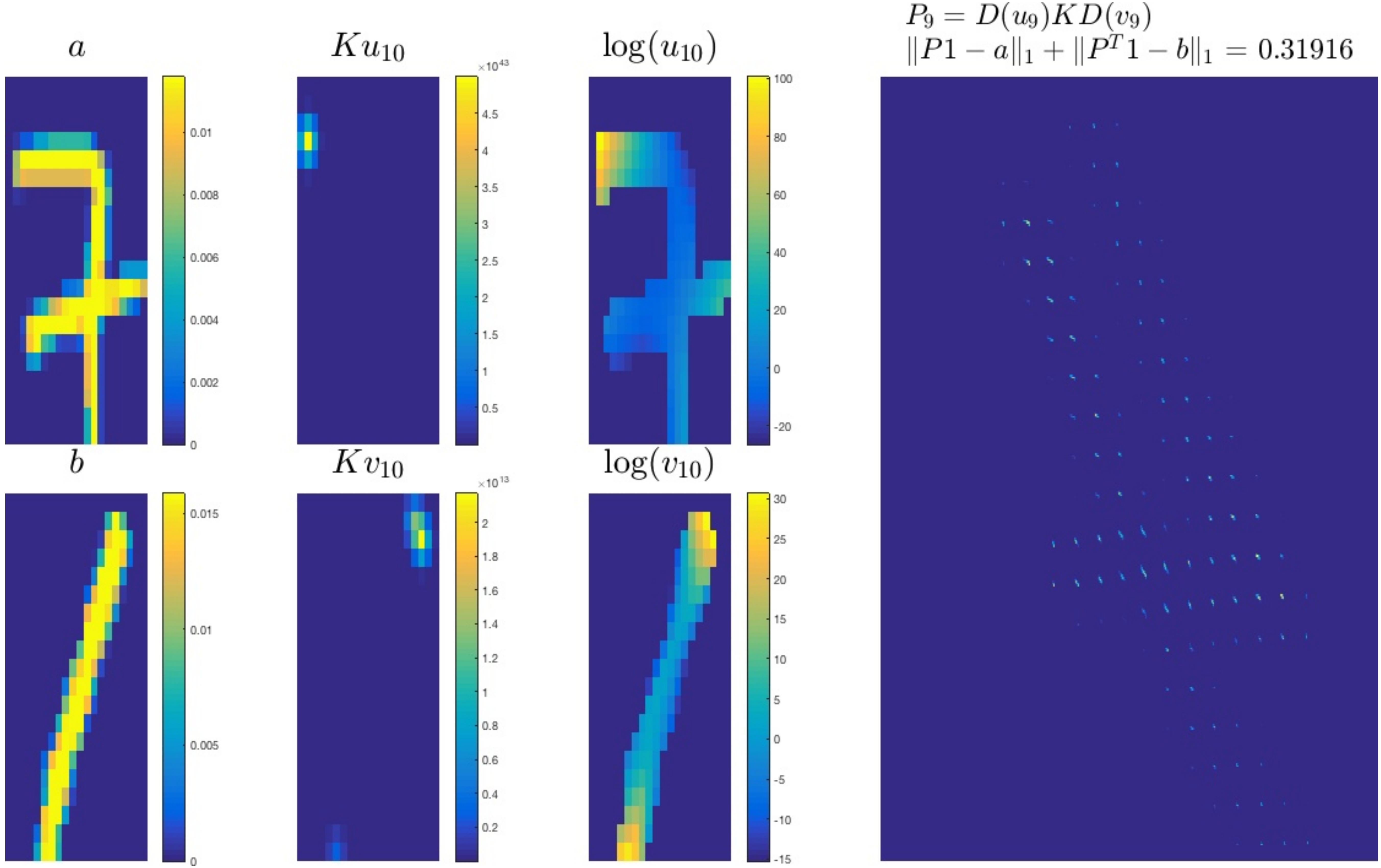


Very Fast EMD Approx. Solver



Very Fast EMD Approx. Solver