Large Scale Machine Learning

European Summer School in Financial Mathematics, Le Mans

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Quick recap on convex optimization

We want to minimize

$$f(\theta) = \frac{1}{n} \sum_{i=1}^{n} f_i(\theta)$$

where $f_i(\theta) = \ell(y_i, \langle x_i, \theta \rangle) + \frac{\lambda}{2} \|\theta\|_2^2$

- Ridge Regression
- Ridge Logistic Regression
- etc.

Quick recap on convex optimization

Full (Batch) Gradient Descent

$$\theta^k \leftarrow \theta^{k-1} - \eta_k \nabla f(\theta^{k-1})$$

You've seen:

- If f convex and L-smooth then for $\eta_k = 1/L$

$$f(\theta^k) - f(\theta_*) \leq \frac{2L\|\theta^0 - \theta_*\|}{k+1} \tag{1}$$

  where $\theta_* \in \operatorname{argmin}_\theta f(\theta)$

- Acceleration (Nesterov, Fista): rate improvement $O(1/k^2)$
- Linesearch

If f is also μ-strongly convex, then linear convergence

$$f(\theta^k) - f(\theta_*) \leq \left(1 - \frac{L}{\mu}\right)^k (f(\theta_0) - f(\theta_*)) \tag{2}$$

Stochastic optimization

What if n (and d) is large?

- Each iteration of a full gradient method has complexity $O(nd)$
- I can't put $n \times d$ floats (32 or 64 bits) in my memory

Size of big data makes a modern computer look old: go back to "old" algorithms

- Idea: in machine learning, objective functions are averages of losses

Stochastic Gradient Descent

If I choose uniformly at random $I \in \{1, \ldots, n\}$, then

$$\mathbb{E}[\nabla f_I(\theta)] = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(\theta) = \nabla f(\theta)$$

- $\nabla f_I(\theta)$ is an *unbiased* but very noisy estimate of the full gradient $\nabla f(\theta)$
- Computation of $\nabla f_I(\theta)$ only requires the I-th line of data ($O(d)$ and smaller for sparse data, see next)

Stochastic Gradient Descent

Stochastic Gradient Descent (SGD) algorithm (Robbins and Monro 1951)

- At each iteration, load a line of data chosen randomly (requires an index for fast random access on the hard drive)
- Compute gradient for this line of data
- Do a descent step, using this gradient, and repeat

Stochastic Gradient Descent

Stochastic Gradient Descent (SGD)

- **Input**: starting point θ^0, sequence of learning rates $\{\eta_t\}_{t\geq 0}$
- For $t = 1, 2, \ldots$ until *convergence* do
  - Pick at random (uniformly) i in $\{1, \ldots, n\}$
  - Put
$$\theta^t = \theta^{t-1} - \eta_t \nabla f_i(\theta^{t-1})$$
- **Return** last θ^t

- Each iteration has complexity $O(d)$ instead of $O(nd)$ for full gradient methods
- Possible to reduce this to $O(s)$ when features are s-sparse using **lazy-updates** (more on this later)

Stochastic Gradient Descent

- Note that if i is chosen uniformly at random in $\{1, \dots, n\}$

$$\mathbb{E}[\nabla f_i(\theta^{t-1}) | \mathcal{F}_{t-1}] = \frac{1}{n} \sum_{i'=1}^{n} \nabla f_{i'}(\theta^{t-1}) = \nabla f(\theta^{t-1})$$

  where $\mathcal{F}_t =$ information until iteration t (relative to random sampling of indexes)
- Namely, SGD uses very noisy unbiased estimations of the full gradient
- Learning rate η_t usually chosen as $\eta_t \approx Ct^{-\alpha}$ with $\alpha \in [1/2, 1]$.
- Linesearch: η_t is a valid learning rate if

$$f_i(\theta^t - \eta_t \nabla f_i(\theta^t)) \leq f_i(\theta^t) - \frac{\eta_t}{2} \|\nabla f_i(\theta^t)\|_2^2$$

Polyak-Ruppert averaging (ASGD)

- Use SGD iterates $\{\theta^t\}$ but return $\bar{\theta}^t = \frac{1}{t}\sum_{t'=1}^{t}\theta^{t'}$
- Computed "online"

$$\bar{\theta}^t \leftarrow \frac{1}{t}\theta^{t-1} + \frac{t-1}{t}\bar{\theta}^{t-1} \tag{3}$$

- Leads to better results, cf:

`http://leon.bottou.org/projects/sgd`

Stochastic Gradient Descent

Theoretical knowledge on SGD. Typical assumptions

- Each f_i is L-smooth (gradient L-lipshitz)
- f is μ-strongly convex
- Non strongly convex: rate $O(1/\sqrt{t})$ for ASGD with $\eta_t = O(1/\sqrt{t})$
- μ-Strongly convex: rate $O(1/(\mu t))$ for ASGD with $\eta_t = O(1/(\mu t))$

Both SGD and ASGD are **slow**. Best case is $O(1/t)$ convergence when f is strongly convex, while $O(e^{-\rho t})$ for FG

Beyond SGD

Recent results improve this:

- Bottou and LeCun (2005)
- Shalev-Shwartz et al (2007, 2009)
- Nesterov et al. (2008, 2009)
- Bach et al. (2011, 2012, 2014, 2015)
- T. Zhang et al. (2014, 2015)

Stochastic vs Batch optimization

- Gradient descent:

$$\theta^t \leftarrow \theta^{t-1} - \frac{\eta_t}{n} \sum_{i=1}^{n} \nabla f_i(\theta^{t-1})$$

  $O(nd)$ iteration but linear convergence $O(e^{-\rho t})$ (strongly cvx case)

- Stochastic gradient descent:

$$\theta^t \leftarrow \theta^{t-1} - \eta_t \nabla f_{i_t}(\theta^{t-1})$$

  $O(d)$ iteration but slow convergence $O(1/t)$ (strongly cvx case)

Do a fast algorithm with $O(d)$ iteration exist?

Variance reduction

- Put $X = \nabla f_I(\theta)$ with I uniformly chosen at random in $\{1, \ldots, n\}$
- We want to use Monte Carlo samples to approximate $\mathbb{E}X = \nabla f(\theta)$
- We find out C s.t. $\mathbb{E}C$ is easy to compute and such that C highly correlated with X
- Put $Z_\alpha = \alpha(X - C) + \mathbb{E}C$ for $\alpha \in [0, 1]$. We have

$$\mathbb{E}Z_\alpha = \alpha\mathbb{E}X + (1 - \alpha)\mathbb{E}C$$

and

$$\operatorname{var} Z_\alpha = \alpha^2(\operatorname{var} X + \operatorname{var} C - 2\operatorname{cov}(X, C))$$

- Standard variance reduction: $\alpha = 1$, so that $\mathbb{E}Z_\alpha = \mathbb{E}X$ (unbiased)

Variance reduction

Idea: combine SGD with variance reduction

$$\theta^t \leftarrow \theta^{t-1} - \eta\Big(\alpha\big(\nabla f_{i_t}(\theta^{t-1}) - \nabla f_{i_t}(\varphi^{t-1})\big) + \frac{1}{n}\sum_{i=1}^{n} \nabla f_i(\varphi^{t-1})\Big)$$

where $\nabla f_i(\varphi^{t-1})$ is the "last computed" gradient of ∇f_i along the iterations

- $\alpha = 1/n$: SAG (Stochastic Average Gradient, Bach et al. 2013)
- $\alpha = 1$: SVRG (Stochastic Variance Reduced Gradient, T. Zhang et al. 2015, 2015)
- $\alpha = 1$: SAGA (Bach et al., 2014)

Variance reduction with SAG

Stochastic Average Gradient (SAG, Bach et al. 2013)

- **Input**: starting point θ_0, learning rate $\eta > 0$
- For $t = 1, 2, \ldots$ until *convergence* do
  - Pick at random (uniformly) i_t in $\{1, \ldots, n\}$
  - Put

$$g_t(i) = \begin{cases} \nabla f_i(\theta^{t-1}) & \text{if } i = i_t \\ g_{t-1}(i) & \text{otherwise} \end{cases}$$

    and compute

$$\theta^t = \theta^{t-1} - \frac{\eta}{n} \sum_{i=1}^{n} g_t(i)$$

- **Return** last θ^t

Variance reduction with SAG

Assume

- Each f_i is L-smooth
- f is μ-strongly convex
- $\eta_t = 1/(16L)$ constant
- Initialize using one epoch of SGD

Non-strongly convex case:

$$\mathbb{E}[f(\theta^t) - f(\theta_*)] \leq O(\frac{\sqrt{n}}{t})$$

Strongly convex case:

$$\mathbb{E}[f(\theta^t) - f(\theta_*)] \leq O\Big(\frac{1}{n\mu} + \frac{L}{n}\Big) \exp\Big(- t\Big(\frac{1}{8n} \wedge \frac{\mu}{16L}\Big)\Big)$$

Improves a lot FG and SGD algorithms

Variance reduction

- Complexity $O(d)$ instead of $O(nd)$ at each iteration
- Choice of a **fixed** step-size $\eta > 0$ possible
- But extra memory required: need to save all the previous gradients.

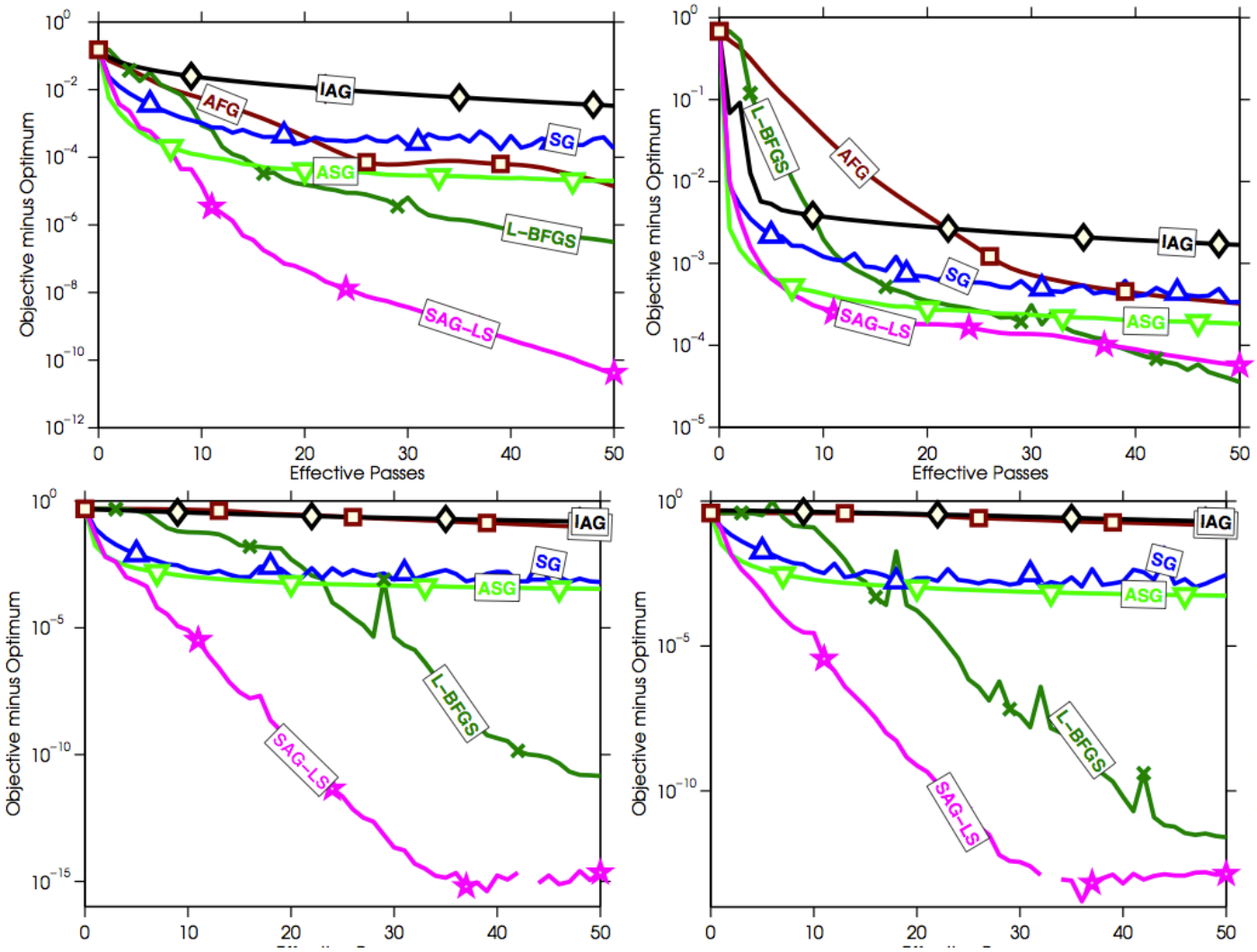
  Hopefully

$$\nabla f_i(\theta) = \ell'(y_i, \langle x_i, \theta \rangle) x_i,$$

  so only need to save $\ell(y_i, \langle x_i, \theta \rangle)$. Memory footprint is $O(n)$ instead of $O(nd)$. If $n = 10^7$, this is 76 Mo

Variance reduction with SAG

Comparison of convergence [Le Roux el al. 2012]



Some practical remarks: file indexing

Now some practical problems / tricks around this

- Need to **index large data files** to be able to read lines at random fast

  Many tools to do this. In `Hadoop`[1] there is the `ArrayFile.Reader` that does that. It's only (roughly) 3x slower than a sequential read of the file.

  Stochastic optimization algorithm also work when using random shuffling of lines at beginning of each epoch: allows to further improve I/O.

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1 hadoop

http://hadoop.apache.org

Some practical remarks: lazy updates

Feature vectors are usually very sparse (words counts). Complexity of the iteration of a stochastic optimization algorithm can reduced from $O(d)$ to $O(s)$, where s is the sparsity of the features. Important since $d \approx 10^6$ while $s \approx 10^3$

For minimizing

$$\frac{1}{n}\sum_{i=1}^{n} \ell(y_i, \langle \theta, x_i \rangle) + \frac{\lambda}{2}\|\theta\|_2^2$$

an iteration of SGD writes

$$\theta^t = (1 - \eta_t \lambda)\theta^{t-1} - \eta_t \ell'(y_i, \langle x_i, \theta^{t-1} \rangle) x_i$$

If x_i is s sparse, then computing $\eta_t \ell'(y_i, \langle x_i, \theta^{t-1} \rangle) x_i$ is $O(s)$, but $(1 - \eta_t \lambda)\theta t - 1$ is $O(d)$ ...

Some practical remarks: lazy updates

Trick: put $\theta^t = s_t \beta^t$, with $s_t \in [0, 1]$ and $s_t = (1 - \eta_t \lambda) s_{t-1}$

$$\theta^t = (1 - \eta_t \lambda)\theta^{t-1} - \eta_t \ell'(y_i, \langle x_i, \theta^{t-1} \rangle) x_i$$

becomes

$$\begin{aligned} s_t \beta^t &= (1 - \eta_t \lambda) s_{t-1} \beta^{t-1} - \eta_t \ell'(y_i, s_{t-1} \langle x_i, \beta^{t-1} \rangle) x_i \\ &= s_t \beta^{t-1} - \eta_t \ell'(y_i, s_{t-1} \langle x_i, \beta^{t-1} \rangle) x_i \end{aligned}$$

so the iteration is now

$$\beta^t = \beta^{t-1} - \frac{\eta_t}{s_t} \ell'(y_i, s_{t-1} \langle x_i, \beta^{t-1} \rangle) x_i$$

which has complexity $O(s)$.

Some practical remarks: lazy updates

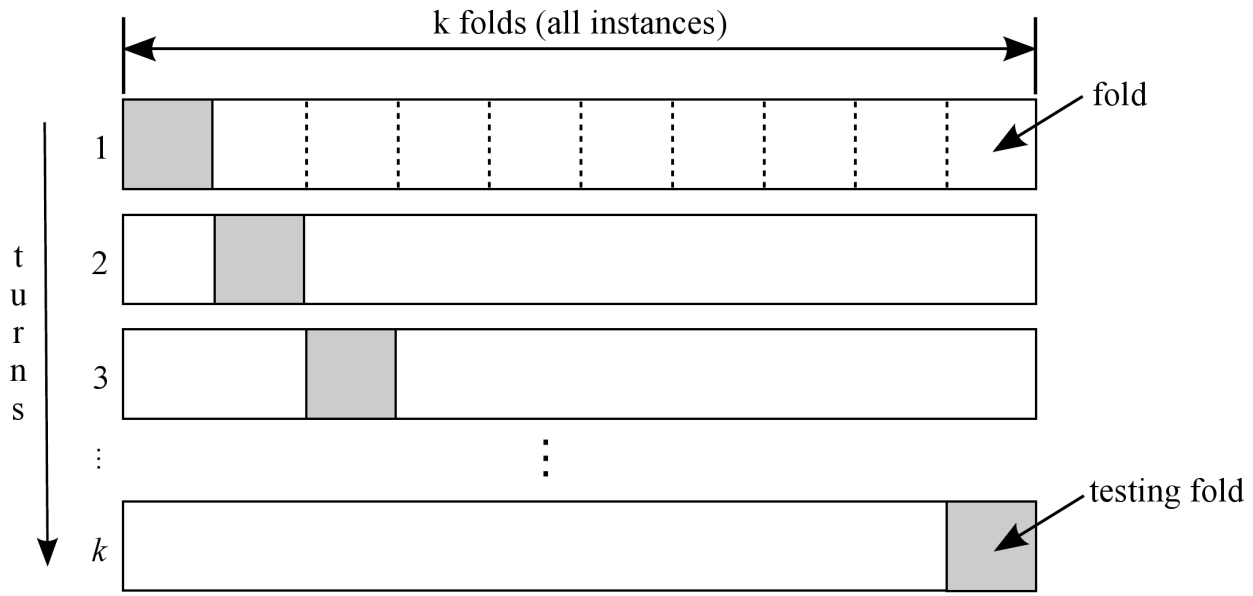
- Just check that s_t is not too small once in a while, in this case put $s_t = 1$ and update θ_t and β_t
- Write the algorithm using only β_t, return $s_t \beta_t$ in the end

Now, complexity of one iteration of a stochastic algorithm is $O(s)$, while an approach based on FG methods is $O(nd)$ without using sparsity

Choice of penalization parameter λ by V-fold with SGD

Quick recap on V-fold:

- Take $V = 5$ or $V = 10$. Pick a random partition $I_1, \ldots, I_V$ of $\{1, \ldots, n\}$, where $|I_v| \approx \frac{n}{V}$ for any $v = 1, \ldots, V$



Some practical remarks: cross-validation

- I don't load the full data in memory
- I can't use V-Fold this way when I'm using an SGD-based solver

Simple solution: when picking a line i at random in the optimization loop, its fold number is given by $i\%V$

- Pick i uniformly at random in $\{1, \ldots, n\}$
- Put $v = i\%V$
- For $v' = 1, \ldots, V$ with $v' \neq v$: Update $\hat{\theta}_{v'}$ using line i
- Update the testing error of $\hat{\theta}_v$ using line i

Cross-validation: warm starting

- So I have many optimization problems to solve for choosing λ!
- If I'm using V-Fold cross-validation, and a choose a set $\Lambda = \{\lambda_1, \ldots, \lambda_M\}$ of values for Λ, it is $V \times |\Lambda|$ problems
- But solutions $\hat{\theta}_{\lambda_{j-1}}$ and $\hat{\theta}_{\lambda_j}$ are going to be close when λ_{j-1} and λ_j are

Use **warm starts**:

- Fix parameters $\lambda_1 < \lambda_2 < \cdots < \lambda_M$
- Put $\theta_0 = 0$ (I don't know where to start)
- For $m = M, \ldots, 1$
  - Put $\lambda = \lambda_m$
  - Solve the problems starting at θ_0 for this value of λ (on each fold)
  - Keep the solutions $\hat{\theta}$ (test it, save it...)
  - Put $\theta_0 \leftarrow \hat{\theta}$

This allows to solve much more rapidly the sequence of problems

Collaborative Filtering

What is collaborative filtering?

Many **users**

Many **items**

- Based on many observed user-item interactions (rating, purchase, click)
- Predict new interactions
- Does Bob like strawberries?

Collaborative Filtering

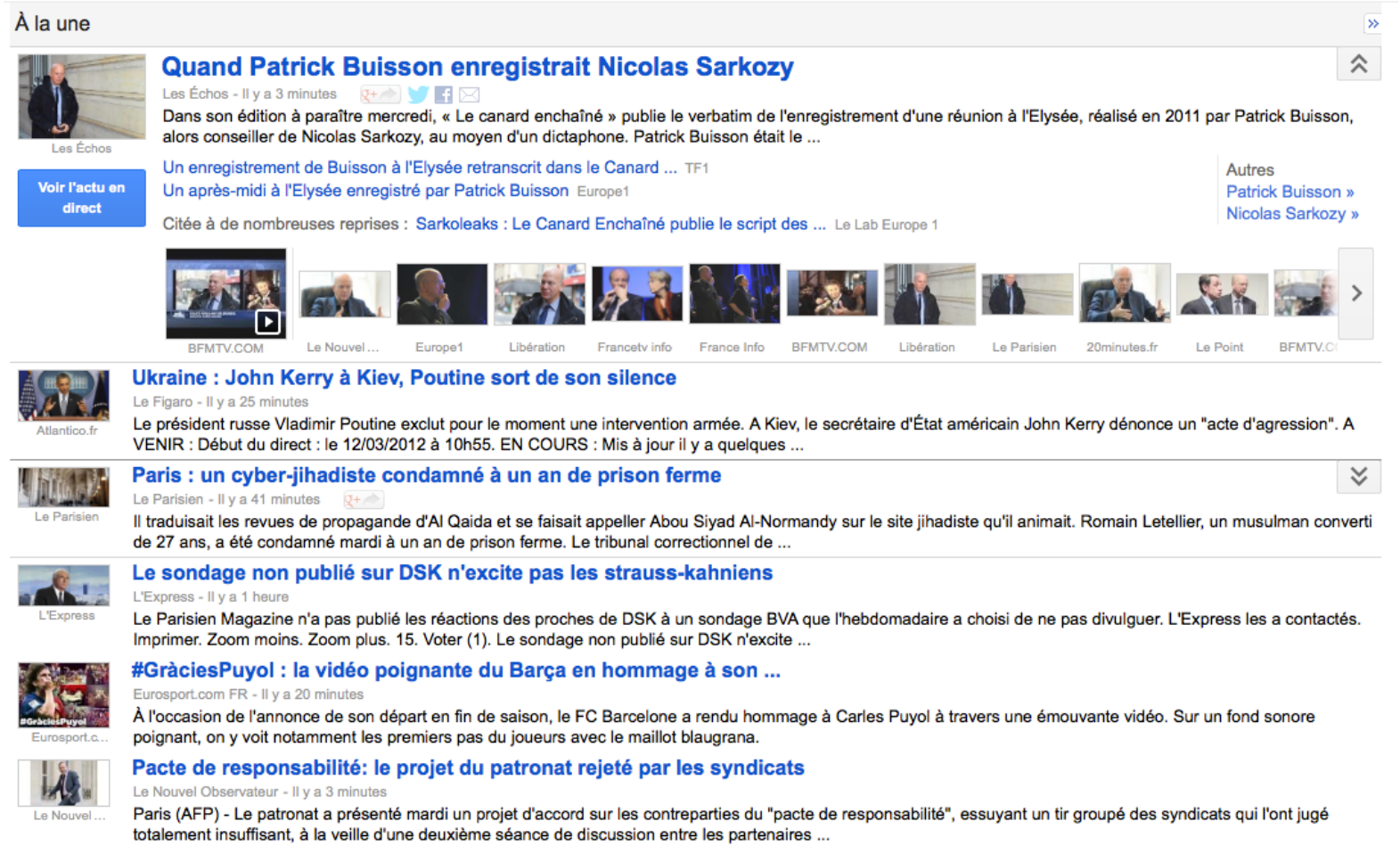
Amazon.com recommends products based on your purchases, browsing history

- but based on the purchases and history of other users too

Collaborative Filtering

Google News recommends news based on your browsing activity

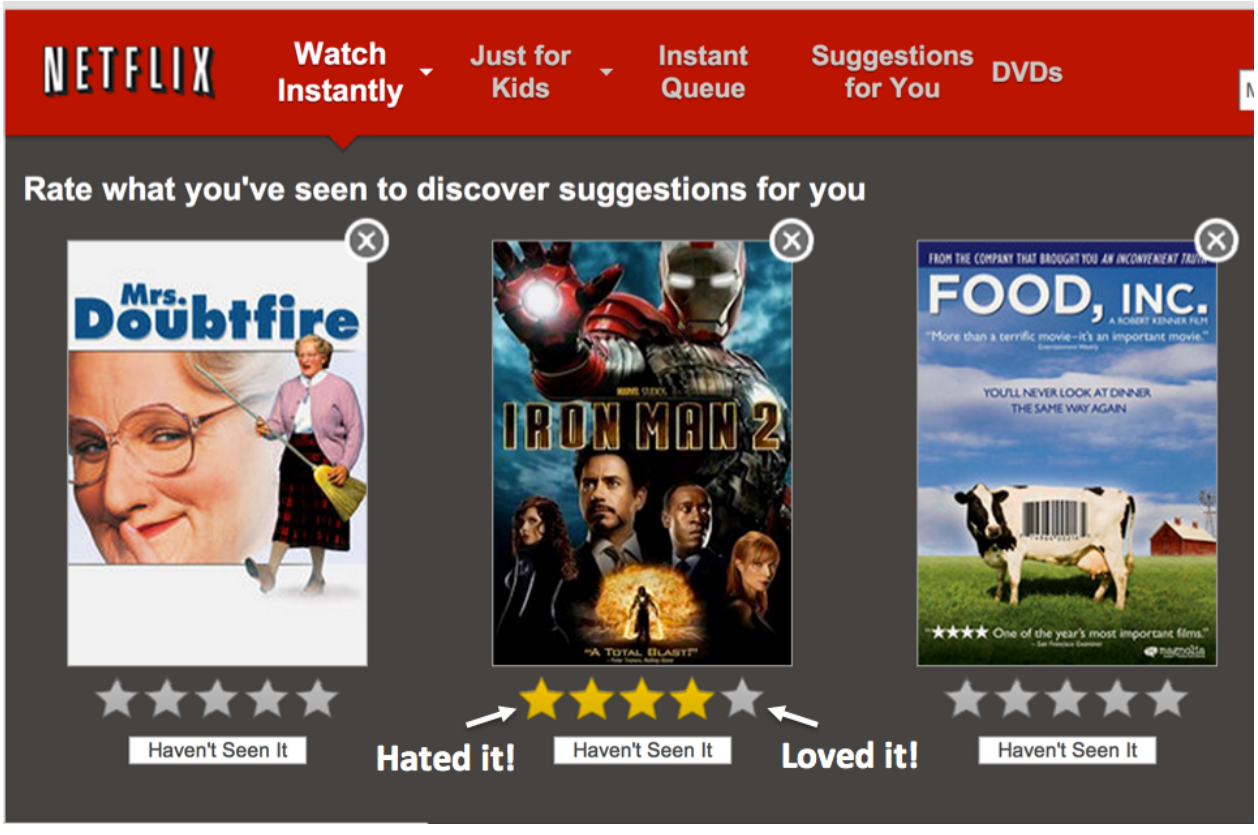
- but on the browsing activity of other users too



Collaborative Filtering

Netflix predicts the rating you'd give to a movie

- using all the ratings given by all users



- 60% of Netflix's DVD rentals due to recommandations

Collaborative Filtering

Netflix predicts the rating you'd give to a movie

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- 60% of Netflix's DVD rentals due to recommandations

Collaborative Filtering: Netflix

Collaborative Filtering: Netflix Prize

Collaborative Filtering: Netflix Prize

Collaborative Filtering: Netflix Prize

Netflix Prize

- October 2, 2006
- Dataset: 100 million ratings , n_U =480K users, n_I =18K movies
- **only 1.1%** of the matrix is filled!
- **Goal**: create a computer code that predicts ratings
- $1m grand prize for anyone beating **Cinematch** accuracy by 10%
- 5000 teams over 150 countries participated

Collaborative Filtering, Matrix completion: **fill unobserved entries** of a matrix

- Unknown matrix M has size $n_U \times n_I$
- Observe $m \ll n_U n_I$ entries (100m $\ll$ 8.64M for Netflix)
- Impossible!

Collaborative Filtering

There is hope:

- Personal preferences are correlated: if Alice likes A and B and Bob likes A, B and C, then Alice is more likely to like C
- There are latent factors that describe the data in a much lower dimensional space. Groups of users, groups of movies, factors that explain the taste of users. High-dimensionality but hidden low-dimensional structure
- The hidden matrix is (approximately) **low-rank**

Collaborative Filtering task:

- discover patterns (low-dimensional hidden structure, latent factors)
- use these patterns for prediction of new user-item interactions
- Do not necessarily use item or user attributes (demographic information, author, genre, cast, plot, etc.)

Given:

- Users $u \in \{1, \ldots, n_U\}$
- Items $i \in \{1, \ldots, n_I\}$
- When u has an interaction with item i, (watches the movie, clicks on a banner, buys a product), he enters a scalar rating $r_{u,i}$ (number of clicks, rating of a movie, etc.)
- Set E of pairs (u, i) of observed ratings $r_{u,i}$

Matrix completion problem

$$M = \begin{bmatrix} ? & ? & 2 & \cdots & 5 \\ 2 & ? & 1 & \cdots & ? \\ ? & 2 & ? & \cdots & 4 \end{bmatrix}$$

Measures of success. Decompose $E = E_{\text{train}} \cup E_{\text{test}}$ into training and testing respectively. $r_{u,i}$ = ground truth and $\hat{r}_{u,i}$ = estimated rating

- Root Mean Square Error

$$\texttt{RMSE} = \sqrt{\frac{1}{|E_{\text{test}}|} \sum_{(u,i) \in E_{\text{test}}} (r_{u,i} - \hat{r}_{u,i})^2}$$

- Mean Absolute Error

$$\texttt{MAE} = \frac{1}{|E_{\text{test}}|} \sum_{(u,i) \in E_{\text{test}}} |r_{u,i} - \hat{r}_{u,i}|$$

- Ranking error: fraction of true top-5 preferences are in my predicted top 5?

Biases

- Remove biases from the ratings
- Some users give systematically higher ratings
- Some items gets systematically better rates (old movies...)
- Don't forget that PCA needs centering

Remove bias

$$\widetilde{r}_{u,i} = r_{u,i} - b_{u,i}$$

Let's denote

- $U(i)$ the set of users who rated item i
- $I(u)$ the set of items rated by user u

Biases

Let's compute means! We can choose $b_{u,i}$ as one of the following:

- Global mean

$$b = \frac{1}{|E|} \sum_{(u,i) \in E} r_{u,i}$$

- Item's mean rating

$$b_i = \frac{1}{|U(i)|} \sum_{u \in U(i)} r_{u,i}$$

- User's mean rating

$$b_u = \frac{1}{|I(u)|} \sum_{i \in I(u)} r_{u,i}$$

- Item's mean rating + user's mean deviation from item mean

$$b_{u,i} = b_i + \frac{1}{|I(u)|} \sum_{i' \in I(u)} (r_{u,i'} - b_{i'})$$

Interpolating means

- Some users have much more ratings than other (1000 $\times$ more!)
- Users with a small numbers of ratings are not as reliable as ones: more noisy. It's hard to trust a mean with only one rating!
- Interpolate between a global estimate and an estimate from user's data

Interpolate to have a better bias estimation:

$$\widetilde{b}_u = \frac{\alpha}{\alpha + |I(u)|} b + \frac{|I(u)|}{\alpha + |I(u)|} b_u$$

where we recall that b is the global mean

$$b = \frac{1}{|E|} \sum_{(u,i) \in E} r_{u,i}$$

and b_u is the user's mean

$$b_u = \frac{1}{|I(u)|} \sum_{} r_{u,i}$$

CF as classification / regression

CF is a set of n_I classifications / regression problem: one for each $i \in \{1, \ldots, n_I\}$

- Consider a fixed i
- Treat each user as a vector (with many missing values) or ratings of all item except i
- The class of each user with respect to i is given by the user's rating
- Prediction of the rating $\hat{r}_{u,i}$ = classication of a user's vector $r_{u,i}$
- Reduces CF to the well-known classification problem
- But, with a huge number of classes!
- This approach does not take advantage of the problem structure

K-NN

K-Nearest Neighbor Method (K-NN) most widely used family of methods

- item-based or user-based
- for product recommandation: **item-based**
- represent each item as a vector of user's ratings with many missing values $r_{\bullet,i} = [2, ?, 1, ?, ?, ?, 2, 1, ?, ?, ?, 5]$

Idea: users rate similar items similarly. In order to predict a rating $r_{u,i}$ for user u and item i:

- Compute similarity between i and every other items
- Find the K items rated by u most similar to i
- Compute weighted average of these ratings

K-NN: Similarity measures

How to measure similarity between items?

- Cosine similarity

$$d(r_{\bullet,i}, r_{\bullet,i'}) = \frac{\langle r_{\bullet,i}, r_{\bullet,i'} \rangle}{\|r_{\bullet,i}\| \|r_{\bullet,i'}\|}$$

- Pearson correlation coefficient

$$d(r_{\bullet,i}, r_{\bullet,i'}) = \frac{\langle r_{\bullet,i} - \bar{r}_{\bullet,i}, r_{\bullet,i'} - \bar{r}_{\bullet,i'} \rangle}{\|r_{\bullet,i} - \bar{r}_{\bullet,i}\| \|r_{\bullet,i'} - \bar{r}_{\bullet,i'}\|}$$

- Inverse Euclidean distance

$$d(r_{\bullet,i}, r_{\bullet,i'}) = \frac{1}{\|r_{\bullet,i} - r_{\bullet,i'}\|}$$

Vectors $r_{\bullet,i}$ contains many missing values: compute these similarities over subets of users that rated both items i and i'

K-NN

How to choose the K-nearest neighbors?

- Select the K items with largest similarity score to item i, among the items rated by u, denoted $N(i, u)$
- Prediction given by

$$\hat{r}_{u,i} = b_{u,i} + \sum_{i' \in N(i,u)} w_{i,j}(r_{u,i'} - b_{u,i'})$$

where $w_{i,i'}$ weights

Example of weights:

- Equal weights

$$w_{i,i'} = \frac{1}{N(u,i)}$$

- Similarity weights

$$w_{i,i'} = \frac{d(r_{\bullet,i}, r_{\bullet,i'})}{\sum_{i'' \in N(i,u)} d(r_{\bullet,i}, r_{\bullet,i''})}$$

Event better: user optimized weights.

- Choose weights that best predict other known ratings of i among all users that rated i
- Corresponds to many small linear regression problems
- Needs to store **many** weights $O(n_I^2)$

Conclusion for K-NN methods

- Easy to implement
- No training time
- Flexible
- But need to store many parameters (all item, vectors, weights in memory)
- Don't exploit hidden low-dimensional structure

MF: if I know the item's features

Matrix Factorization (= MF)

- Assume that we know features about the items

$$y_i = [\text{cast}, \text{year}, \text{genre}, \cdots] \in \mathbb{R}^r$$

  for all $i = 1, \ldots, n_I$.
- r features for each item
- We want the users parameters x_u for $u = 1, \ldots, n_U$

Linear regression

$$\hat{x}_u \in \operatorname*{argmin}_{x_u} \sum_{i \in I(u)} (r_{u,i} - \langle x_u, y_i \rangle)^2.$$

Even better: **ridge regression**

$$\hat{x}_u = \operatorname*{argmin}_{x_u} \sum_{i \in I(u)} (r_{u,i} - \langle x_u, y_i \rangle)^2 + \lambda \|x_u\|_2^2$$

- But we don't want to construct ad-hoc features y_i for items
- Not a good idea for building recommandations

MF: if I know the user's features

- Assume that we know user's features x_u for all $u = 1, \ldots, n_U$.
- r features for each user
- We want the items features y_i for $i = 1, \ldots, n_I$

Once again: **linear regression**

$$\hat{y}_i \in \operatorname*{argmin}_{y_i} \sum_{u \in U(i)} (r_{u,i} - \langle x_u, y_i \rangle)^2.$$

Even better: **ridge regression**

$$\hat{y}_i \in \operatorname*{argmin}_{y_i} \sum_{u \in U(i)} (r_{u,i} - \langle x_u, y_i \rangle)^2 + \lambda \|y_i\|_2^2$$

- But we can't construct ad-hoc features x_u for users
- Still not a good idea for building recommandations

MF: put everything together

- We don't want to construct ad-hoc features y_i for items
- We can't construct ad-hoc features x_u for users

So let's learn items and users features **at the same time**!

- Putting things together

$$\hat{x}_u = \underset{x_u}{\operatorname{argmin}} \sum_{i \in I(u)} (r_{u,i} - \langle x_u, \hat{y}_i \rangle)^2 + \lambda \|x_u\|_2^2$$

$$\hat{y}_i = \underset{y_i}{\operatorname{argmin}} \sum_{u \in U(i)} (r_{u,i} - \langle \hat{x}_u, y_i \rangle)^2 + \lambda \|y_i\|_2^2$$

for all $u = 1, \ldots, n_U$ and $i = 1, \ldots, n_I$

MF: put everything together

$$\hat{x}_u = \underset{x_u}{\operatorname{argmin}} \sum_{i \in I(u)} (r_{u,i} - \langle x_u, \hat{y}_i \rangle)^2 + \lambda \|x_u\|_2^2$$

$$\hat{y}_i = \underset{y_i}{\operatorname{argmin}} \sum_{u \in U(i)} (r_{u,i} - \langle \hat{x}_u, y_i \rangle)^2 + \lambda \|y_i\|_2^2$$

for all $u = 1, \ldots, n_U$ and $i = 1, \ldots, n_I$

- Hum... the $\hat{x}_u$'s depends on the $\hat{y}_i$'s that depend on the $\hat{x}_u$'s that depends on the $\hat{y}_i$ that... !

MF: put everything together

Let's rewrite this. Put

$$X^\top = \begin{bmatrix} \vdots & \vdots & \vdots \\ x_1 & \cdots & x_{n_U} \\ \vdots & \vdots & \vdots \end{bmatrix} \quad \text{and} \quad Y^\top = \begin{bmatrix} \vdots & \vdots & \vdots \\ y_1 & \cdots & y_{n_I} \\ \vdots & \vdots & \vdots \end{bmatrix}$$

Then we consider the minimization of

$$F(X, Y) = \sum_{(u,i)\in E} (r_{u,i} - \langle x_u, y_i \rangle)^2 + \lambda \sum_{u=1}^{n_U} \|x_u\|_2^2 + \lambda \sum_{i=1}^{n_I} \|y_i\|_2^2$$

over $X \in \mathbb{R}^{n_U \times r}$ and $Y \in \mathbb{R}^{n_I \times r}$ jointly.

- The penalization terms $\lambda \sum_{u=1}^{n_U} \|x_u\|_2^2 + \lambda \sum_{i=1}^{n_I} \|y_i\|_2^2$ counters overfitting

$$F(X,Y) = \sum_{(u,i)\in E} (r_{u,i} - \langle x_u, y_i \rangle)^2 + \lambda \sum_{u=1}^{n_U} \|x_u\|_2^2 + \lambda \sum_{i=1}^{n_I} \|y_i\|_2^2$$

over $X \in \mathbb{R}^{n_U \times r}$ and $Y \in \mathbb{R}^{n_I \times r}$ jointly.
Let's write this matricially:

$$F(X,Y) = \|\mathcal{P}_E(R - XY^\top)\|_F^2 + \lambda \|X\|_F^2 + \lambda \|Y\|_F^2$$

where

$$\|A\|_F = \text{ Frobenius norm of } A = \sqrt{\sum_{j,k} A_{j,k}^2}$$

and

$$\mathcal{P}_E(A) = \begin{cases} A_{u,i} & \text{if } (u,i) \in E \\ 0 & \text{otherwise} \end{cases}$$

Put $\lambda = 0$ and $E = \{1, \ldots, n_U\} \times \{1, \ldots, n_I\}$

$$F(X, Y) = \|\mathcal{P}_E(R - XY^\top)\|_F^2 = \|R - XY^\top\|_F^2$$

Solution is given by the SVD (Singular Value Decomposition)
Recall that

- X of size $n_U \times r$
- Y of size $n_I \times r$

Then

$$\underset{X,Y}{\operatorname{argmin}} \|R - XY^\top\|_F^2$$

is given by thresholded SVD of R

SVD (Singular Value Decomposition)

Any matrix $R \in \mathbb{R}^{n_U \times n_I}$ writes

$$R = U \Sigma V^\top$$

where

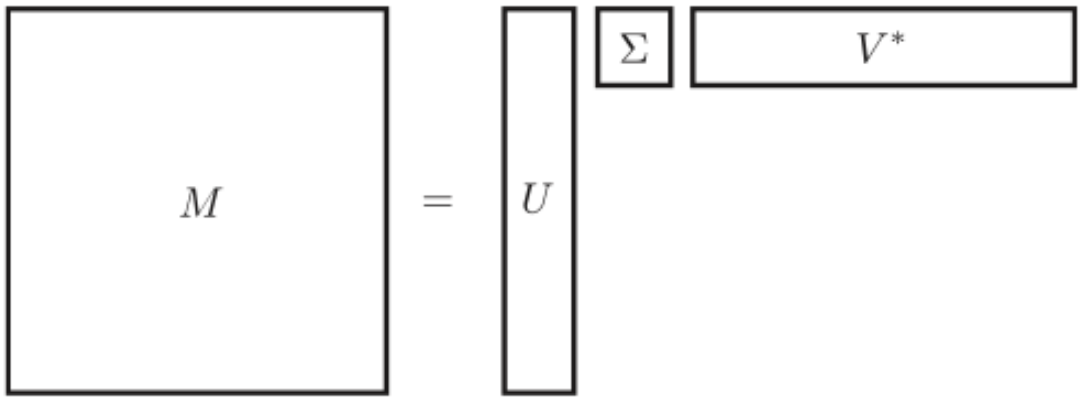
- U is the matrix of **left singular vectors** (columns of U are eigenvectors of $RR^\top$, it satisfies $U^\top U = I$
- V is the matrix of **right singular vectors** (eigenvectors of $R^\top R$, it satisfies $V^\top V = I$
- $\Sigma = \text{diag}[\sigma_1, \ldots, \sigma_{n_U \wedge n_I}]$ is the diagonal matrix containing the **singular values**

  $$\sigma_1 \geq \cdots \geq \sigma_{n_U \wedge n_I}$$

  where

  $$\sigma_j(X) = \sqrt{\lambda_j(X^\top X)} = j\text{th eigenvalue of } X^\top X$$

Matrix Factorization: SVD



Fundamental result:

$$\underset{M \in \mathbb{R}^{n_U \times n_I} : \text{rank}(X) = r}{\text{argmin}} \|R - M\|_2^2 = U_r \Sigma_r V_r^\top$$

where $R = U \Sigma V^\top$ is the SVD of R and

- $\Sigma_r = \text{diag}[\sigma_1, \ldots \sigma_r]$
- U_r contains the first r columns of U
- V_r contains the first r columns of V

- Don't forget that PCA = SVD of the covariance matrix

Matrix Factorization: SVD

Hence a solution of

$$(\hat{X}, \hat{Y}) \in \underset{X,Y}{\operatorname{argmin}} \|R - XY^\top\|_F^2$$

is given by

$$\hat{X} = U_r \Sigma_r \quad \text{and} \quad \hat{Y} = V_r^\top$$

- Matrix completion can be understood as an SVD with missing entries
- With extra regularization to avoid overfitting using ridge penalization

Ok. So how do I solve

$$F(X,Y) = \sum_{(u,i)\in E} (r_{u,i} - \langle x_u, y_i \rangle)^2 + \lambda \sum_{u=1}^{n_U} \|x_u\|_2^2 + \lambda \sum_{i=1}^{n_I} \|y_i\|_2^2$$

or equivalently

$$F(X,Y) = \|\mathcal{P}_E(R - XY^\top)\|_F^2 + \lambda \|X\|_F^2 + \lambda \|Y\|_F^2$$

???

Algorithm 1. Alternating Least-Squares (ALS)

Idea: if we knew Y we could solve X using ridge regression and vice-versa: alternate between optimizing on X and Y with the other matrix fixed

Alternating least-squares (ALS) algorithm

Repeat until *convergence*:

- For each u solve the linear system:
  $x_u^{\text{new}} \leftarrow$ solution of $\sum_{i \in I(u)} (y_i y_i^\top + \lambda I) x_u = \sum_{i \in I(u)} r_{u,i} y_i$
- For each item i solve
  $y_i^{\text{new}} \leftarrow$ solution of $\sum_{u \in U(i)} (x_u x_u^\top + \lambda I) y_i = \sum_{u \in U(i)} r_{u,i} x_u$
- $x_u \leftarrow x_u^{\text{new}}$, $y_i \leftarrow y_i^{\text{new}}$

- Updates for x_u and y_i can be done in parallel
- Complexity. Space: $O(n_u r + n_I r)$ and time: $O(n_u r^3 + n_I r^3)$ per iteration. $O(r^3)$ for solving the linear systems
- No need to store the complete ratings matrix

Algorithm 2. Gradient Descent (GD)

Idea: use standard gradient descent

- $\nabla_{x_u} F(X, Y) = \lambda x_u + \sum_{i \in I(u)} (\langle x_u, y_i \rangle - r_{u,i}) y_i$
- $\nabla_{y_i} F(X, Y) = \lambda y_i + \sum_{u \in U(i)} (\langle x_u, y_i \rangle - r_{u,i}) x_u$

Gradient Descent algorithm

Repeat until *convergence*:

- For each u update
  $x_u^{\text{new}} \leftarrow x_u - \eta \left(\lambda x_u + \sum_{i \in I(u)} (\langle x_u, y_i \rangle - r_{u,i}) y_i \right)$
- For each i update
  $y_i^{\text{new}} \leftarrow y_i - \eta \left(\lambda y_i + \sum_{u \in U(i)} (\langle x_u, y_i \rangle - r_{u,i}) x_u \right)$
- $x_u \leftarrow x_u^{\text{new}}$, $y_i \leftarrow y_i^{\text{new}}$

- Updates for x_u and y_i can be done in parallel
- Complexity: $O(n_u r + n_I r)$ no $O(r^3)$ overhead iteration
- No need to store the complete ratings matrix

Algorithm 3. Stochastic Gradient Descent (SGD)

Stochastic Gradient Descent algorithm

Repeat until *convergence*:

- Choose $(u, i) \in E$ at random
- Update x_u
  $x_u^{\text{new}} \leftarrow x_u - \eta(\lambda x_u + (\langle x_u, y_i \rangle - r_{u,i})y_i)$
- Update y_i
  $y_i^{\text{new}} \leftarrow y_i - \eta(\lambda y_i + (\langle x_u, y_i \rangle - r_{u,i})x_u)$
- $x_u \leftarrow x_u^{\text{new}}$, $y_i \leftarrow y_i^{\text{new}}$

- Complexity: $O(n_u r + n_I r)$ no $O(r^3)$ overhead iteration
- No need to store the complete ratings matrix

Conclusion for CF using Matrix Factorization

Parameters to tune:

- step-size, or learning rate η. Must be decreasing for SGD
- Regularization parameter $\lambda > 0$ and number of latent factors r. Tuned using cross-validation

There is a big problem:

$$F(X, Y) = \sum_{(u,i)\in E} (r_{u,i} - \langle x_u, y_i \rangle)^2 + \lambda \sum_{u=1}^{n_U} \|x_u\|_2^2 + \lambda \sum_{i=1}^{n_I} \|y_i\|_2^2$$

is **not** a convex problem

- Local minimum, initialization is important
- No guarantees towards a good minimum
- Mostly heuristics

A convex formulation of the matrix completion problem

- Unknown matrix R of size $n_U \times n_I$
- If R has rank r, its degrees of freedom are $r(n_U + n_I - r)$
- $E \subset \{1, \dots, n_U\} \times \{1, \dots, n_I\}$ of observed entries of R
- We need $|E| \geq r(n_U + n_I - r)$ (otherwise no hope to recover R
- We observe only $\mathcal{P}_E(R)$

We assume that the rank of R is small. So let's penalize the rank

- Tempting to consider

$$\hat{R} \in \operatorname*{argmin}_{M \in \mathbb{R}^{n_U \times n_I}} \left\{ \frac{1}{2} \|\mathcal{P}_E(M - R)\|_F^2 + \lambda \operatorname{rank}(M) \right\}$$

- Too hard
- For Lasso we've found that a convex relaxation of ℓ_0 is ℓ_1
- Can't we do the same for the rank?

Yes!

A convex formulation of the matrix completion problem

$$\text{rank}(M) = \sum_{k=1}^{n_U \wedge n_I} \mathbf{1}_{\sigma_j(M)>0} = \|\sigma(M)\|_0$$

Replace ℓ_0 by ℓ_1:

$$\|M\|_* = \sum_{j=1}^{n_I \wedge n_U} \sigma_j(M)$$

Hence tempting to consider

$$\hat{R} \in \underset{M \in \mathbb{R}^{n_I \times n_U}}{\text{argmin}} \left\{ \frac{1}{2} \|\mathcal{P}_E(M - R)\|_2^2 + \lambda \|M\|_* \right\}$$

for a regularization parameter $\lambda > 0$. This is a **convex** problem!

Proximal gradient descent

Proximal gradient descent for the CF problem

Repeat until *convergence*:

- $M \leftarrow S_{\lambda\eta_k}(M - \eta_k(\mathcal{P}_E(M - R)))$

where S_λ is the spectral soft-thresholding operator: if $M = U\Sigma V^\top$ SVD of M, then

$$S_\lambda(M) = U\,\mathrm{diag}[(\sigma_1 - \lambda)_+, \ldots, (\sigma_{n_1 \wedge n_2} - \lambda)_+]V^\top$$

Thresholding of the singular value: the solution will be of low rank. Many other algorithms, more memory efficient and faster

Proximal gradient descent

- Convex problem: convex optimization and convergence guarantees to a minimum
- Bottleneck: an SVD is necessary at **each iteration**! Complexity of an SVD $O((n_U \vee n_I)(n_U \wedge n_I)^2)$
- Can be reduced using partial SVD (compute only k top singular values and vectors). Complexity is (best case) $O(n_1 n_2 k)$ [keyword: **Lanczos** algorithms]
- Compute an approximate solution, given some tolerance
- For remedy for large SVD is the **divide and conquer** principle

Sketch of application: image inpainting

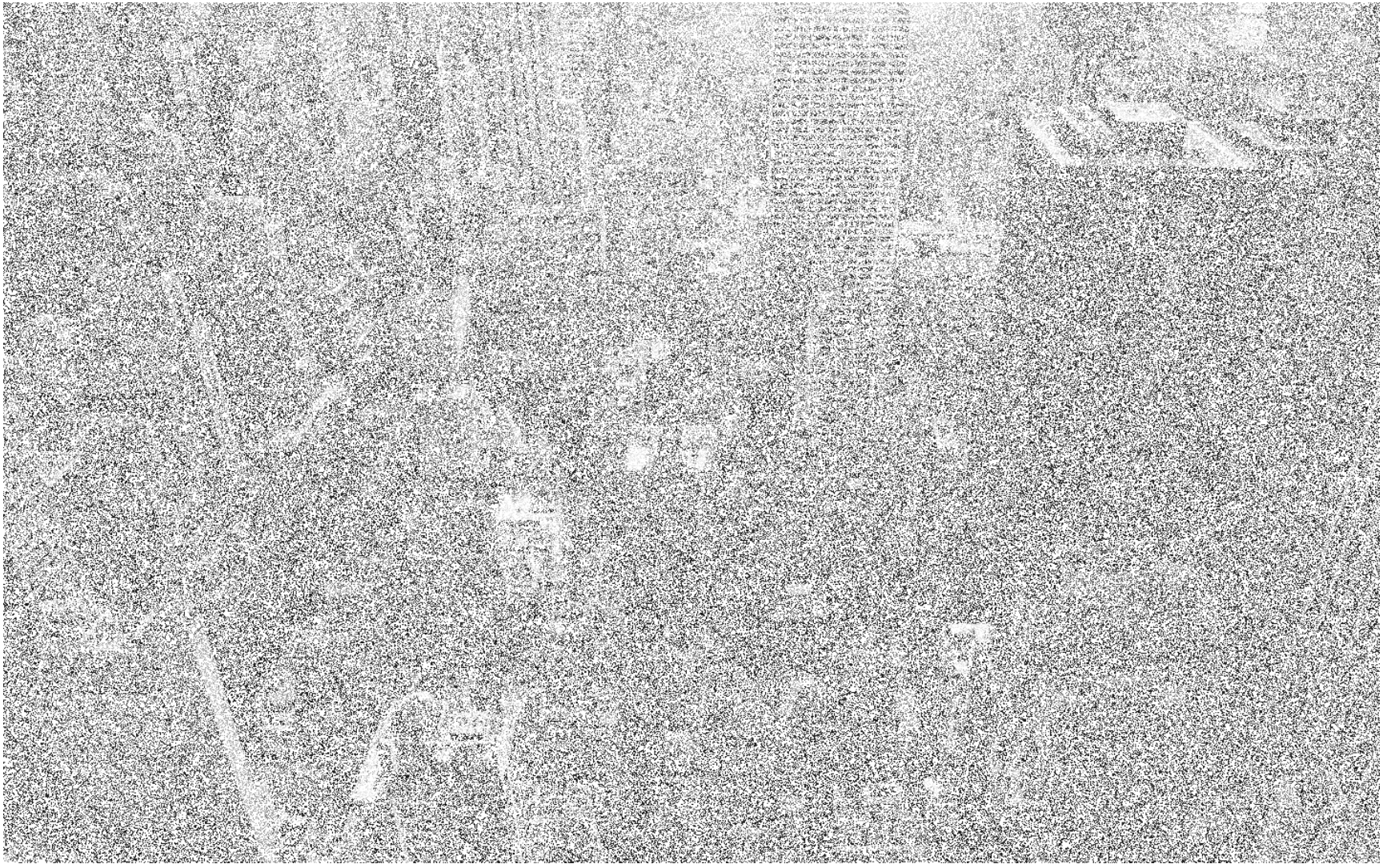
Sketch of application: image inpainting

Sketch of application: image inpainting

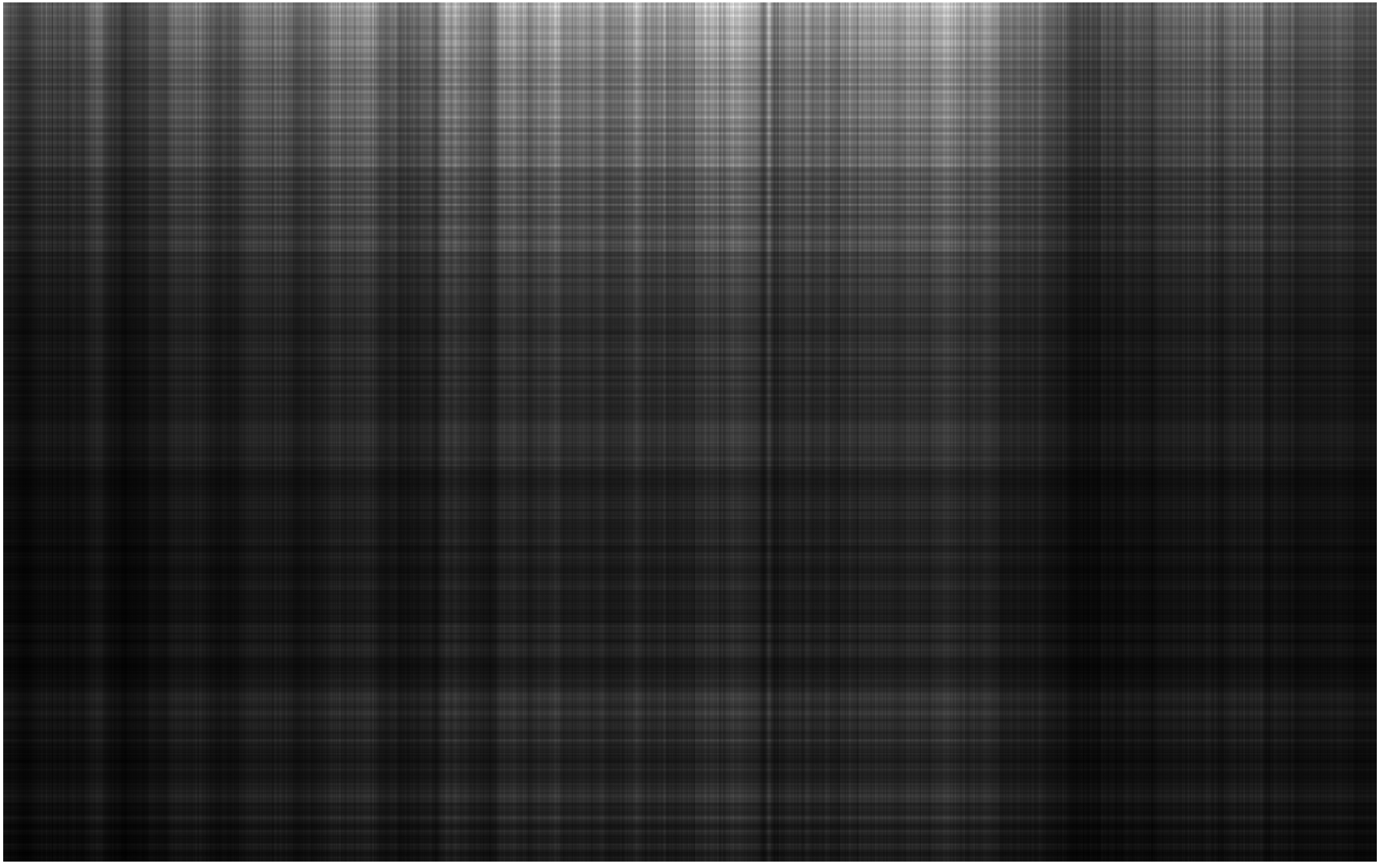
Sketch of application: image inpainting

Sketch of application: matrix completion

We only observe 35% of the picture



Collaborative Filtering, Matrix Completion



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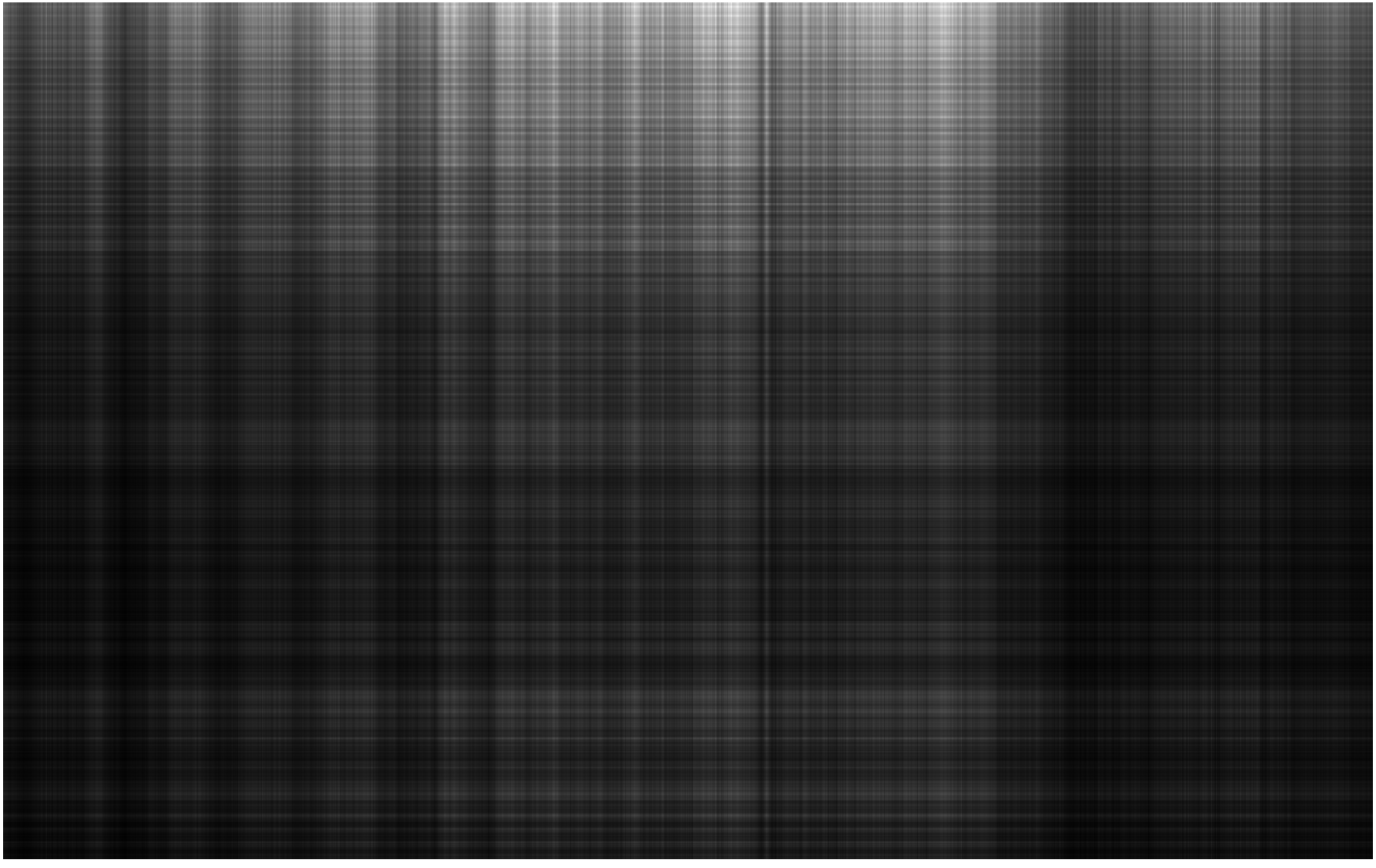

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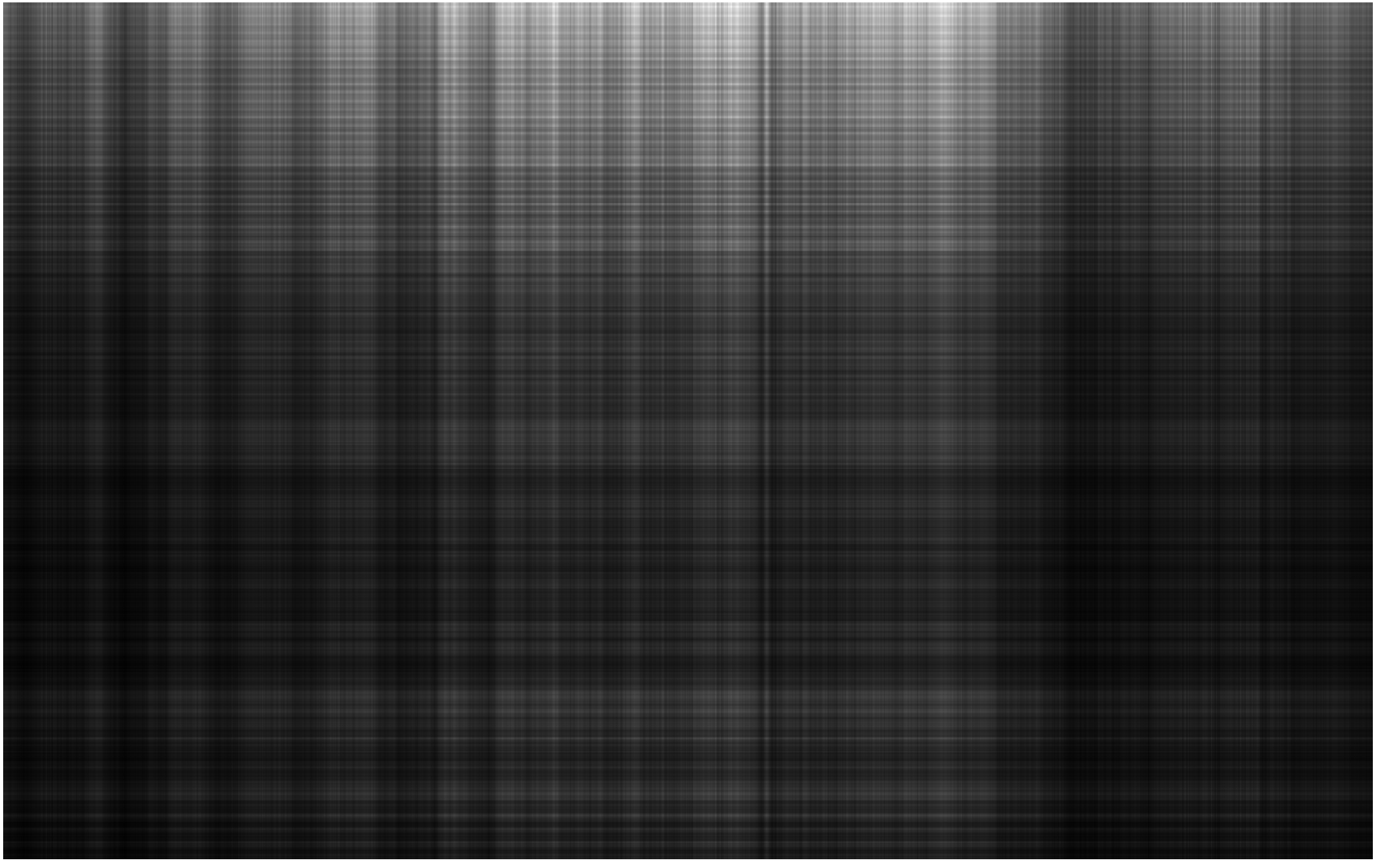

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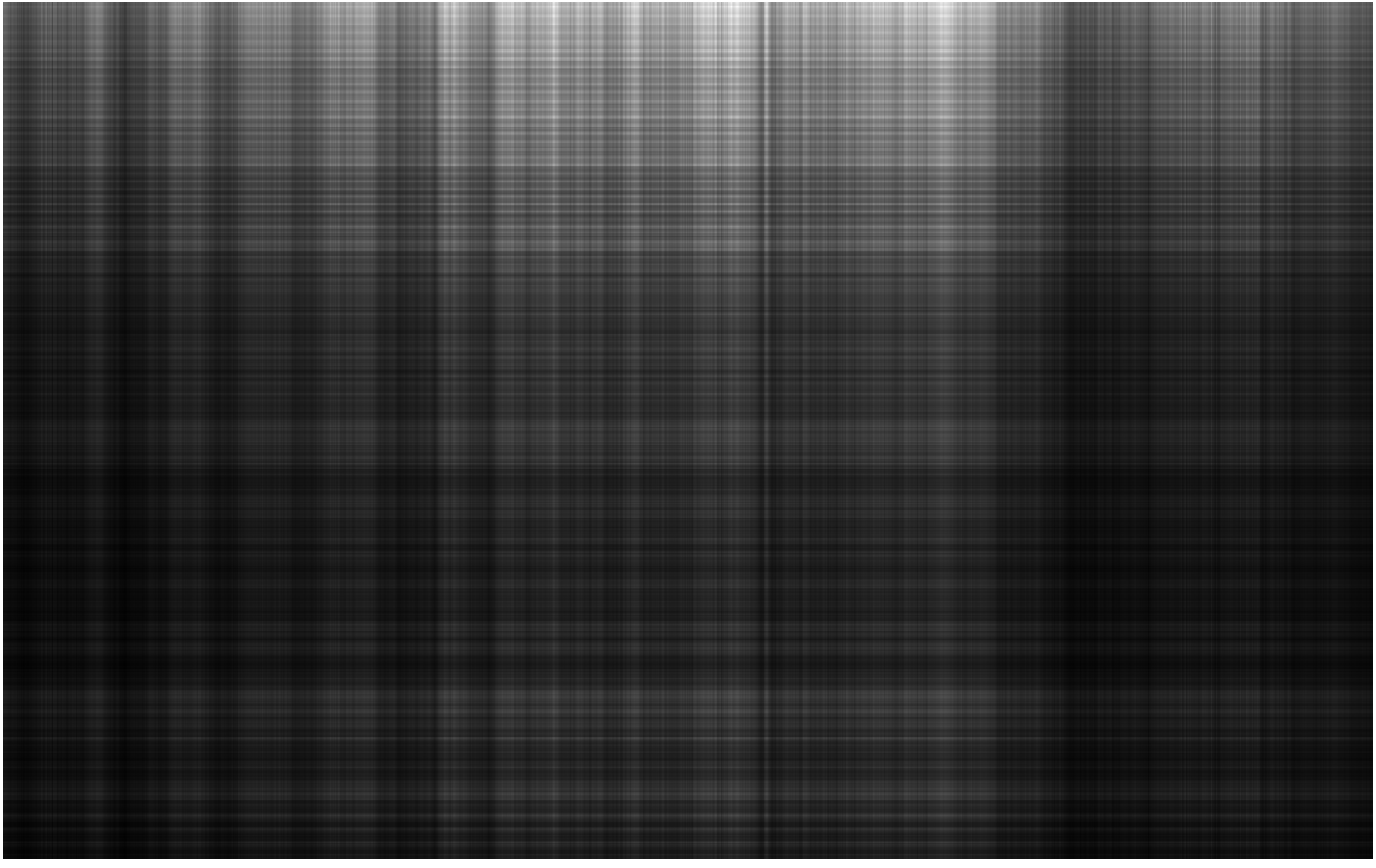

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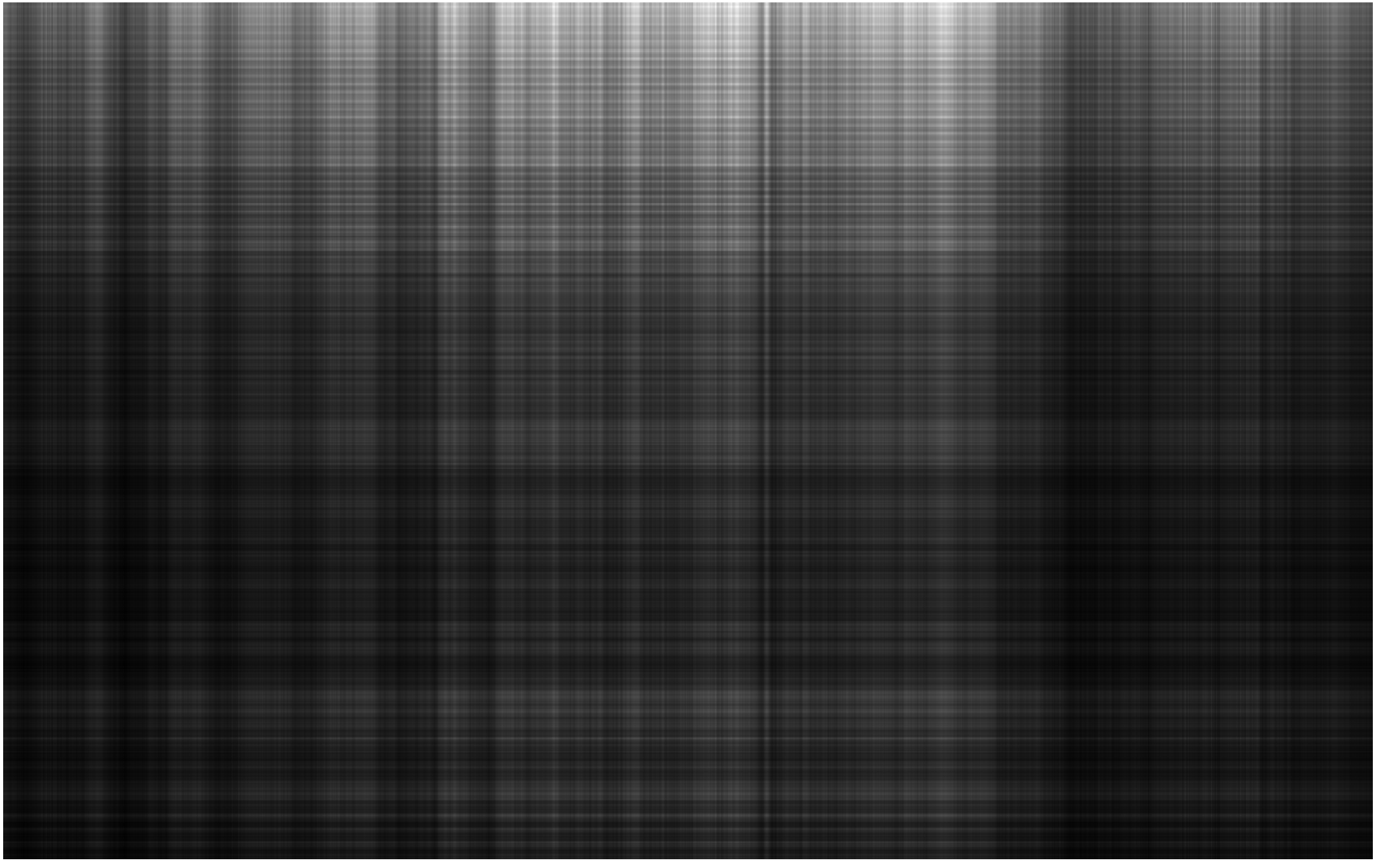

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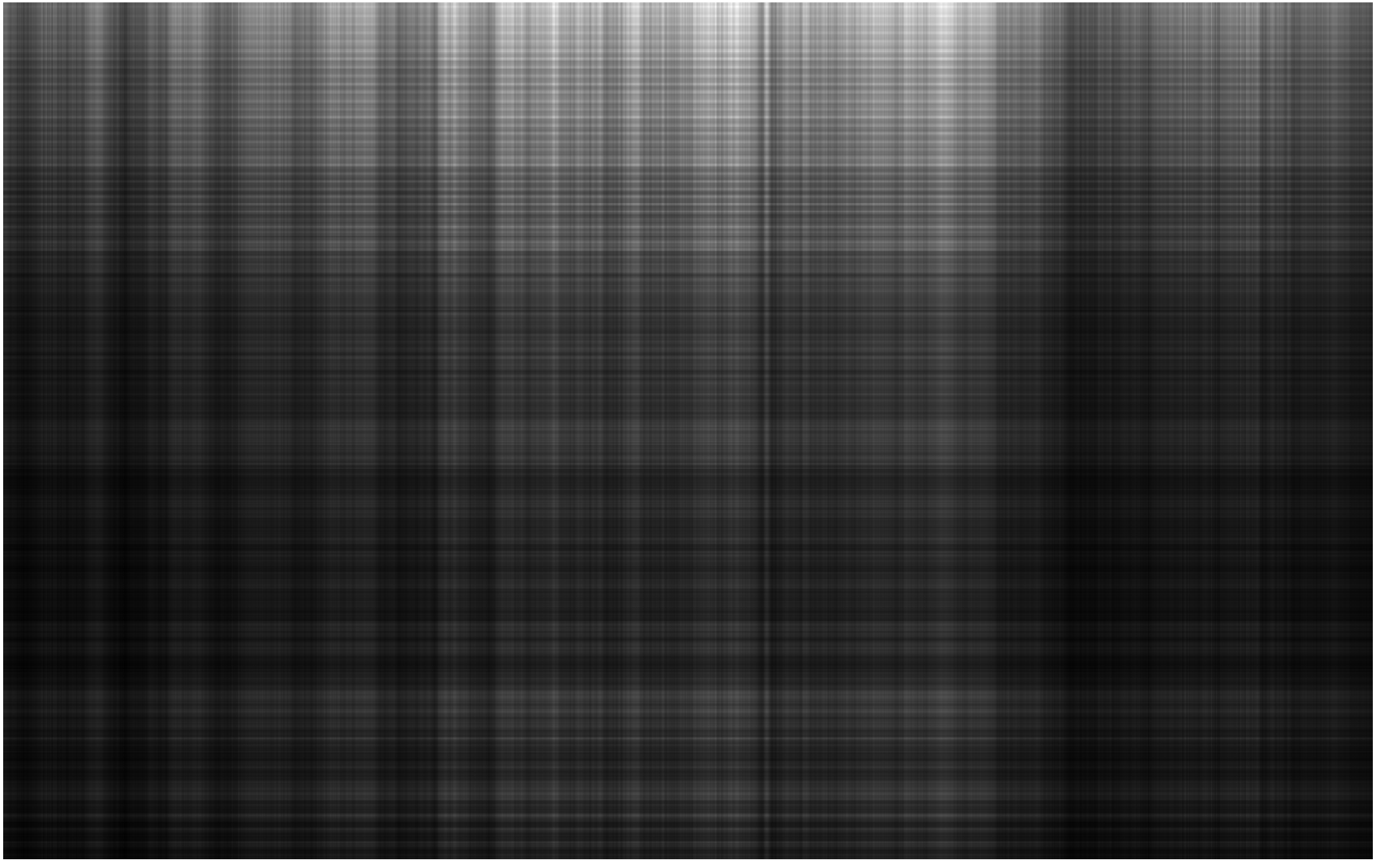

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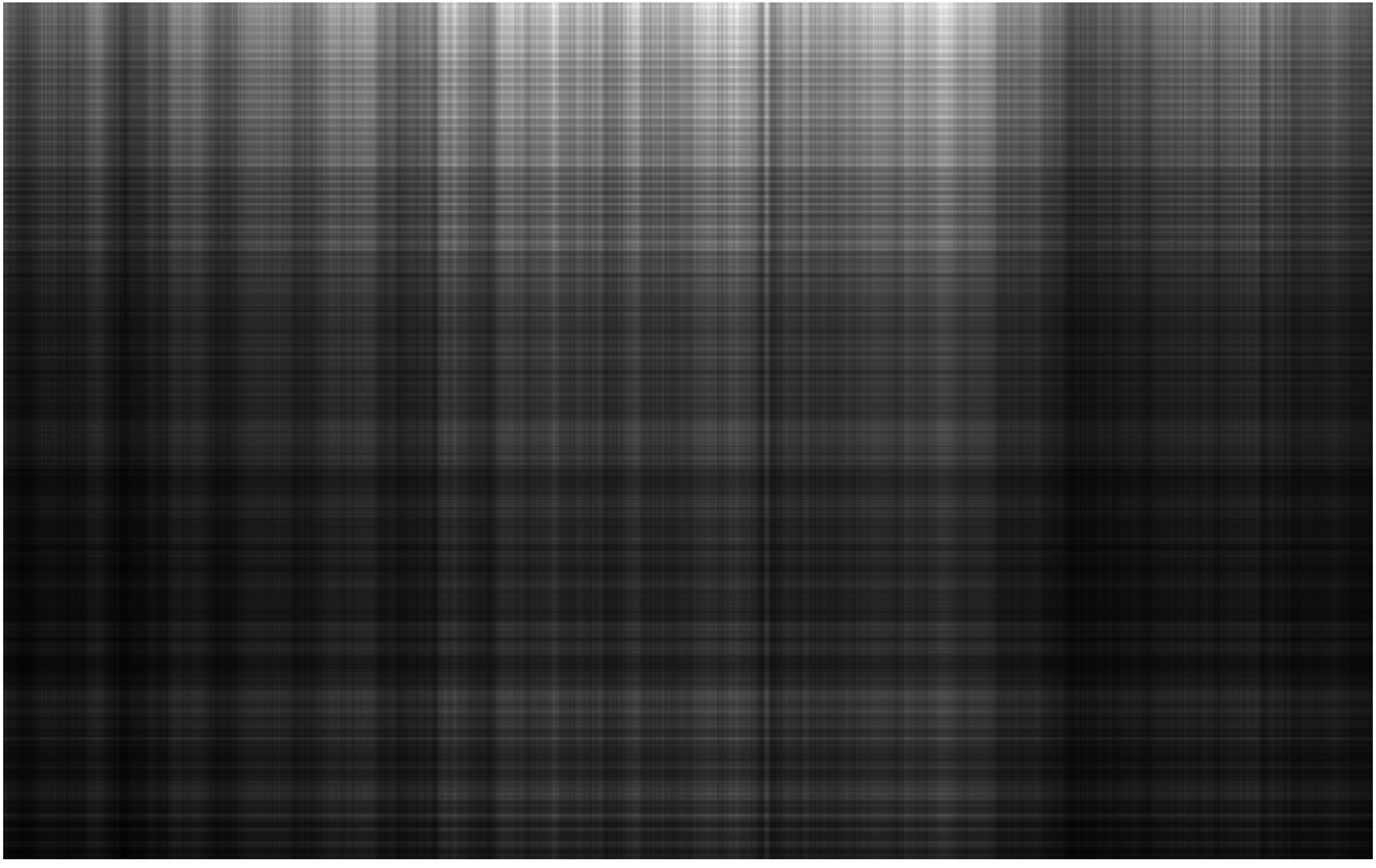

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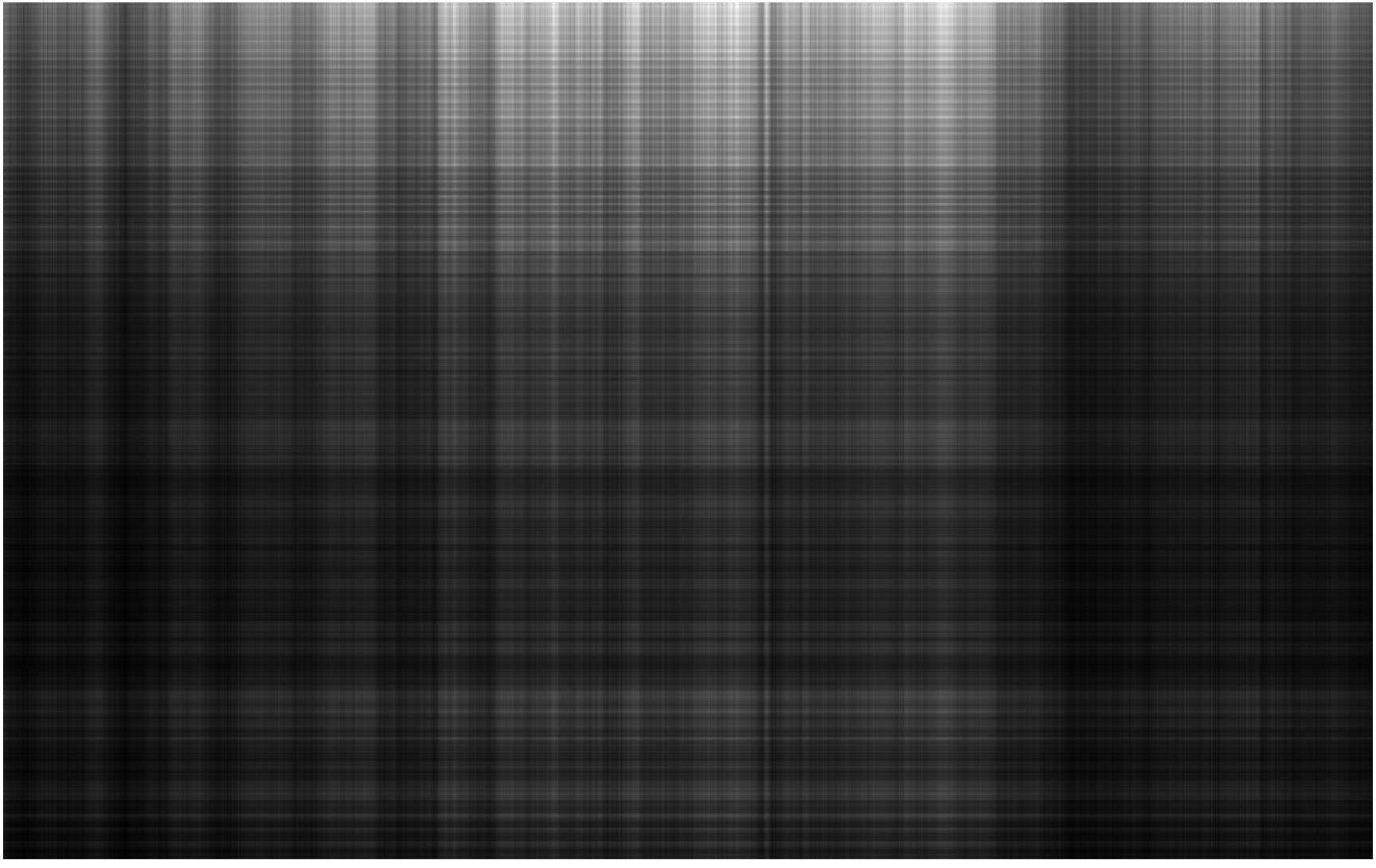

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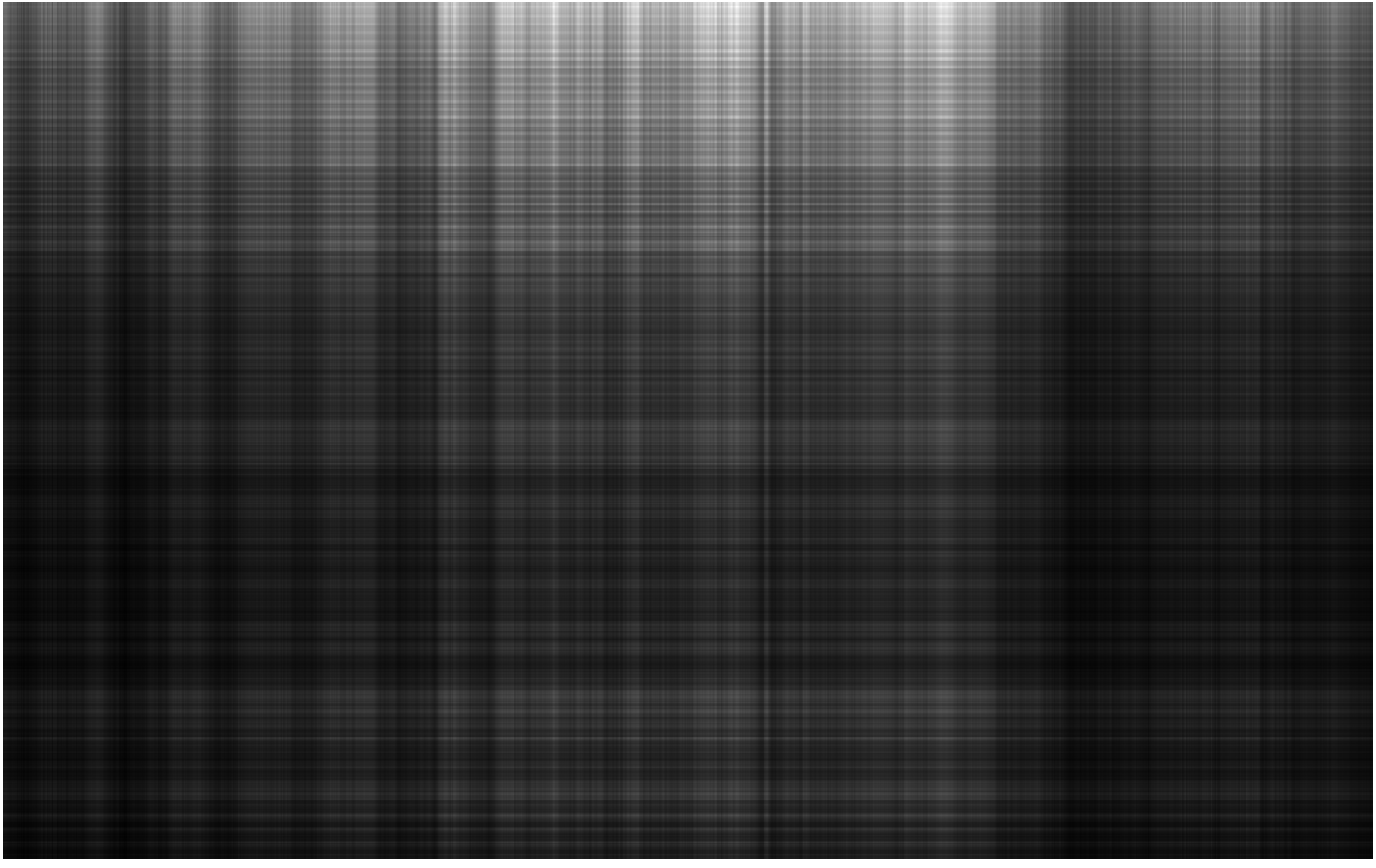

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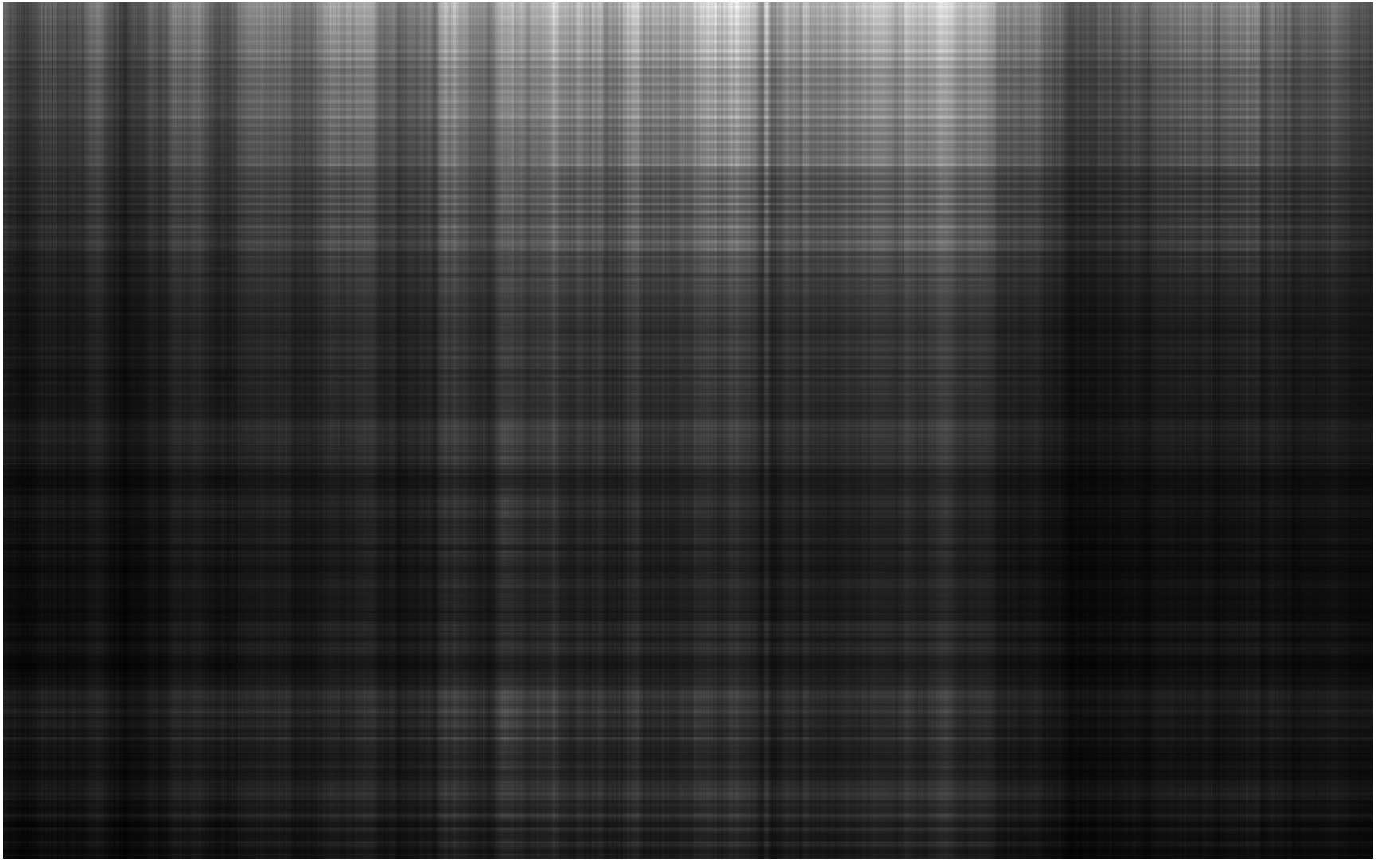

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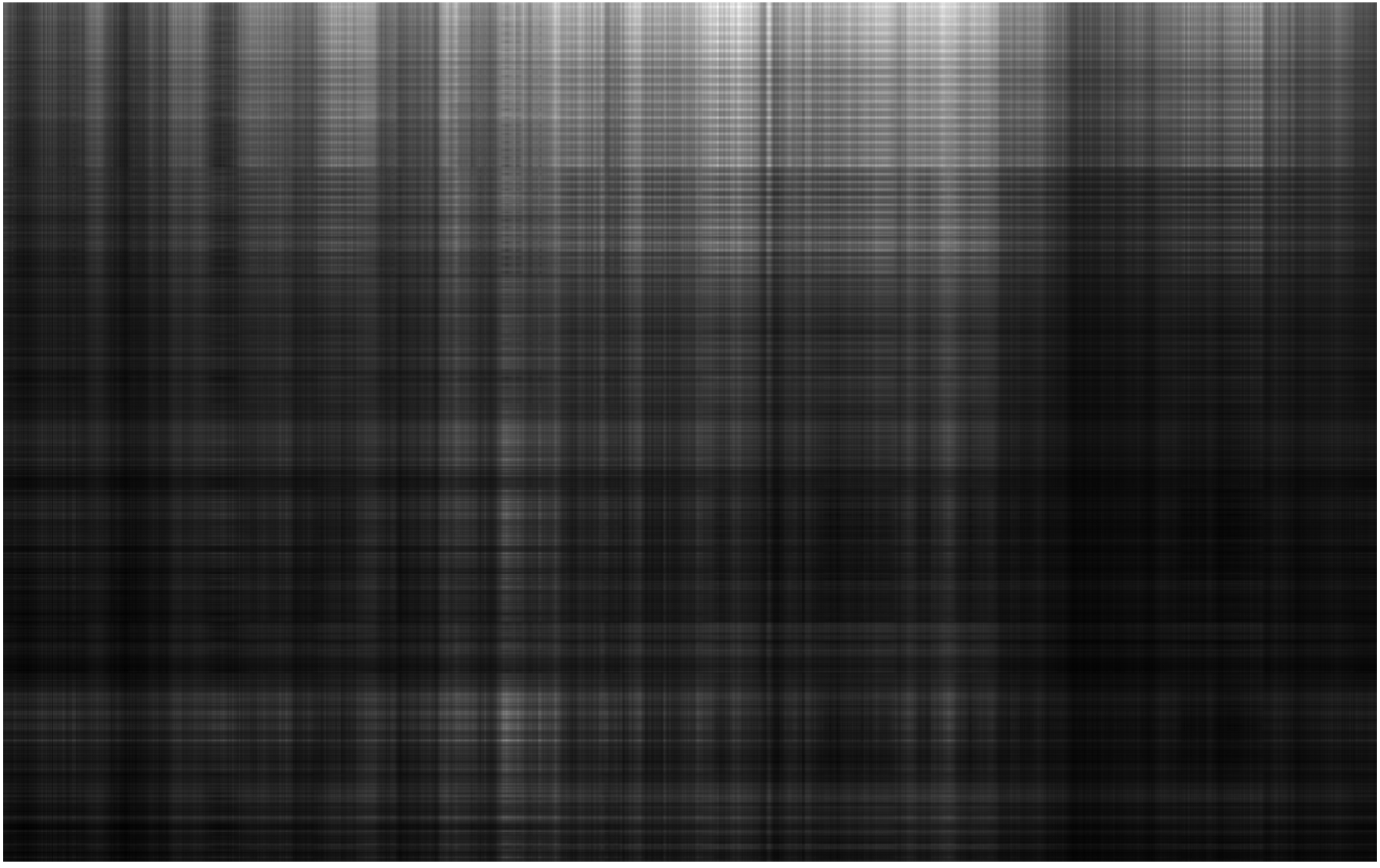

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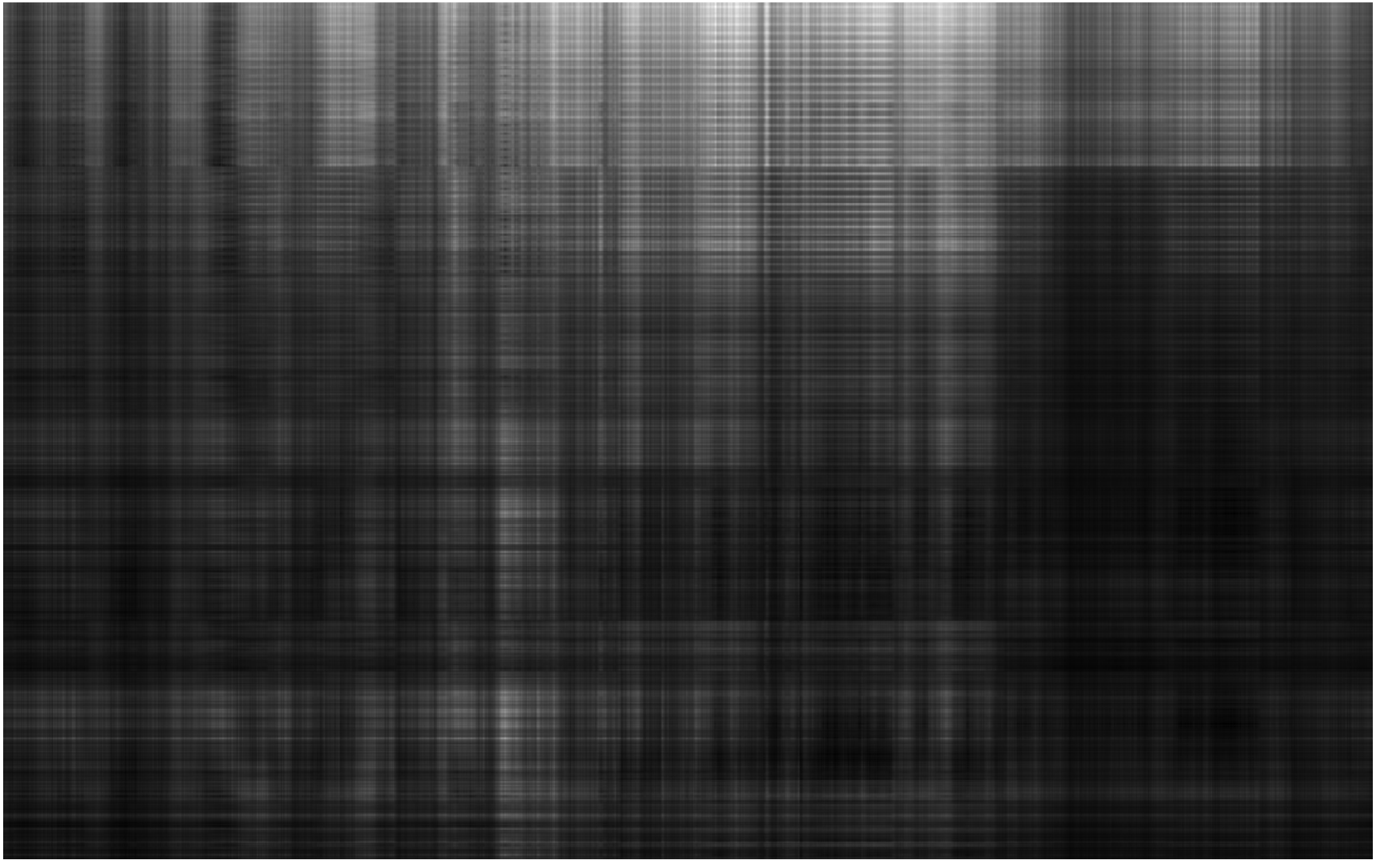

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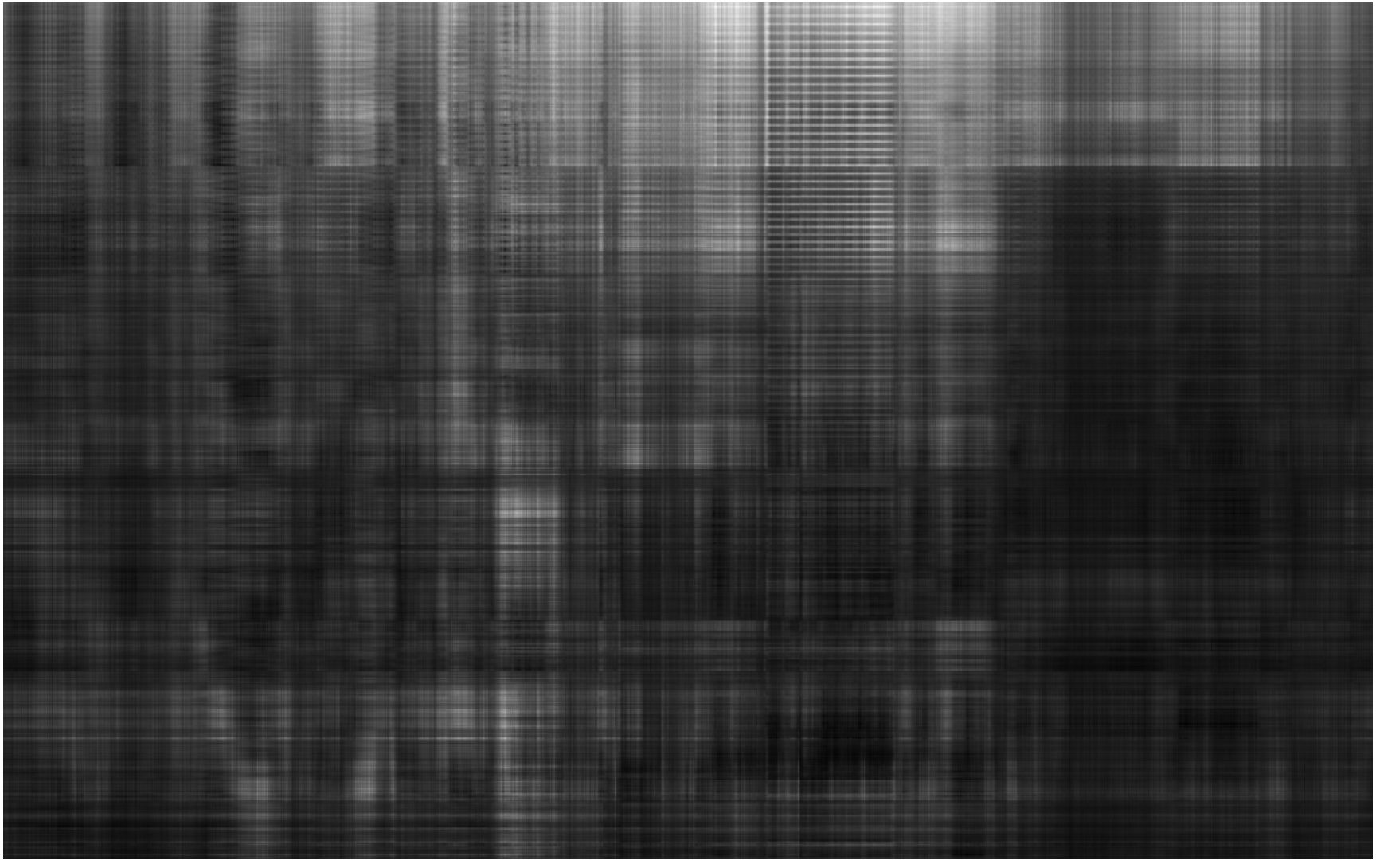

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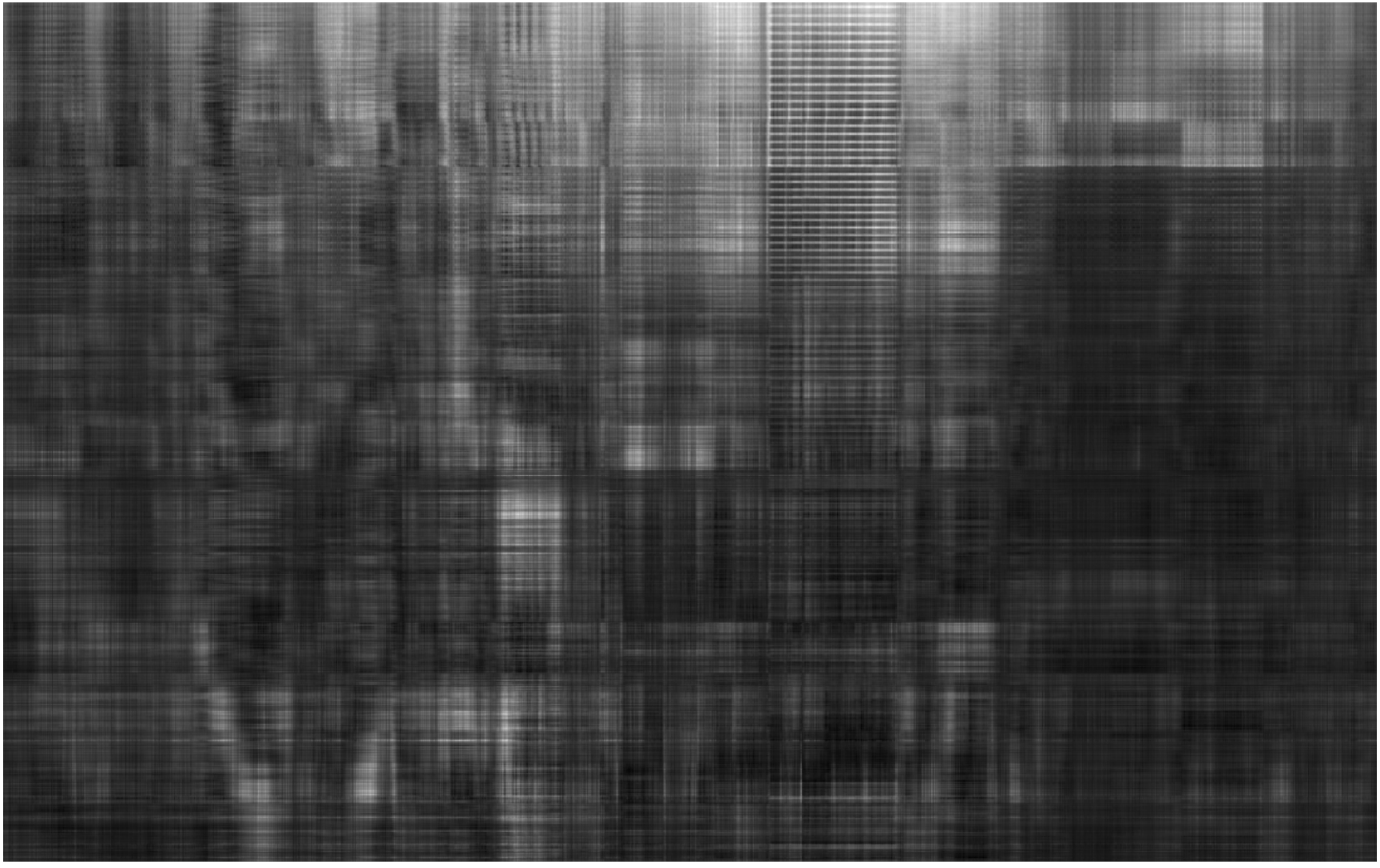

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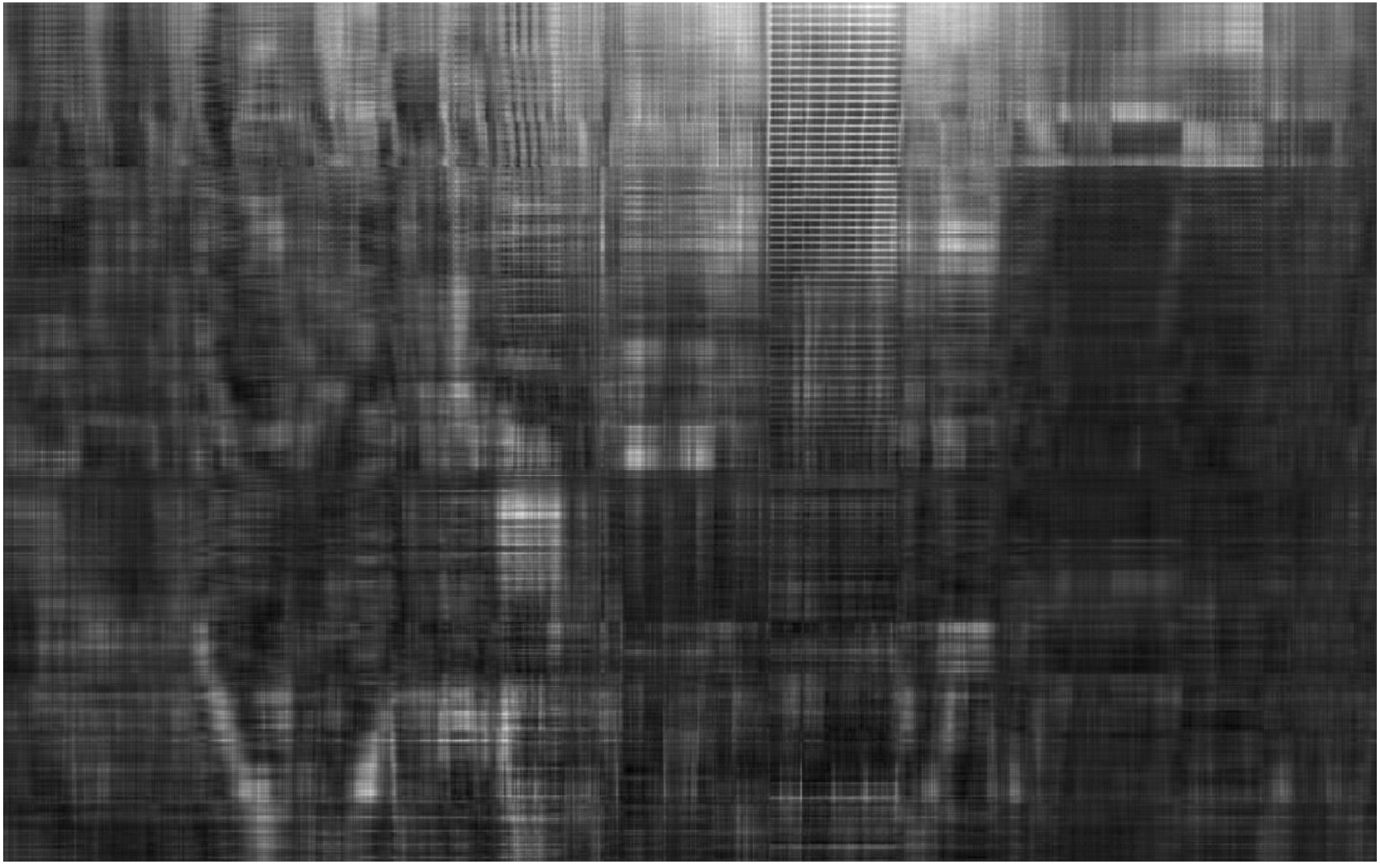

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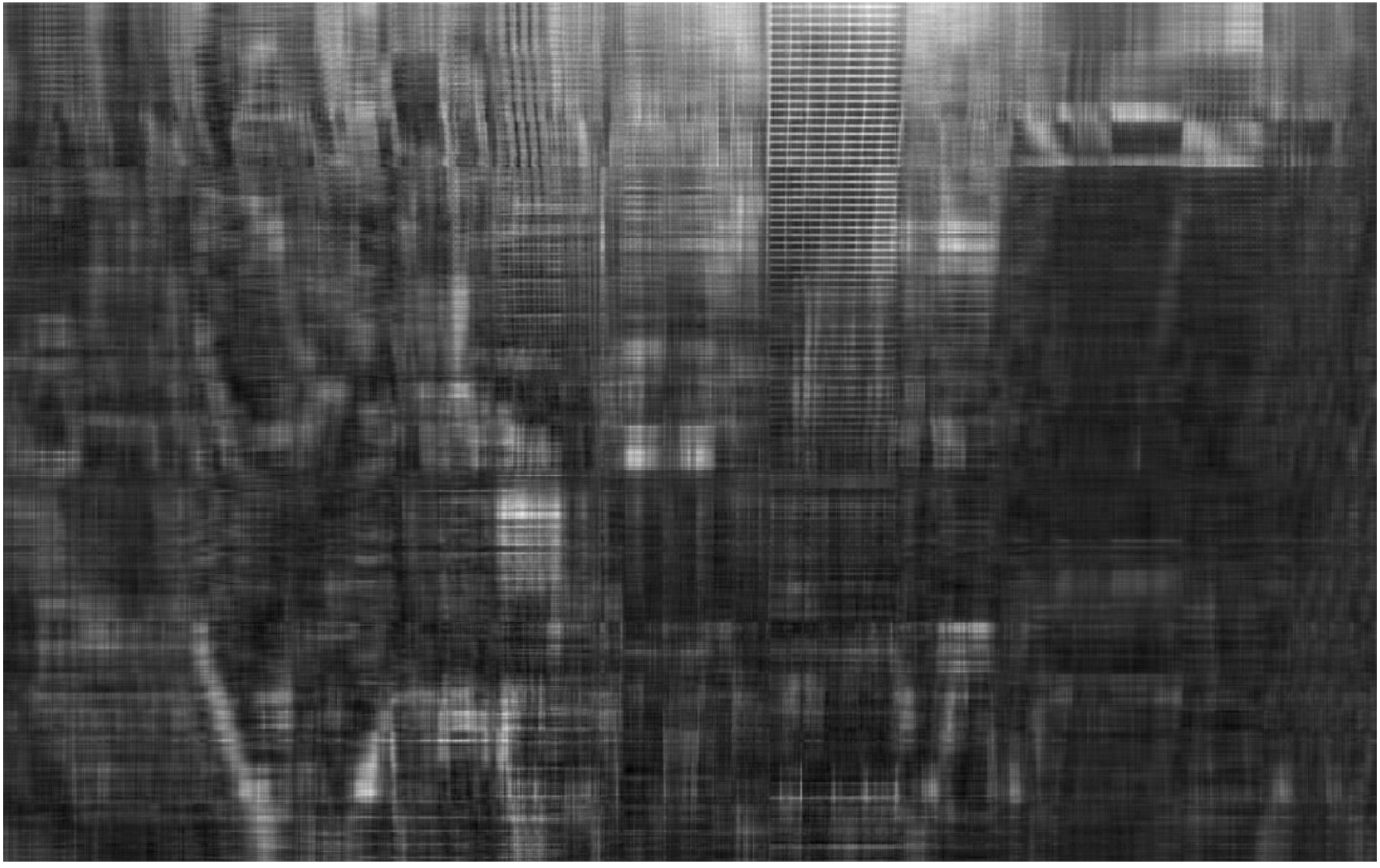

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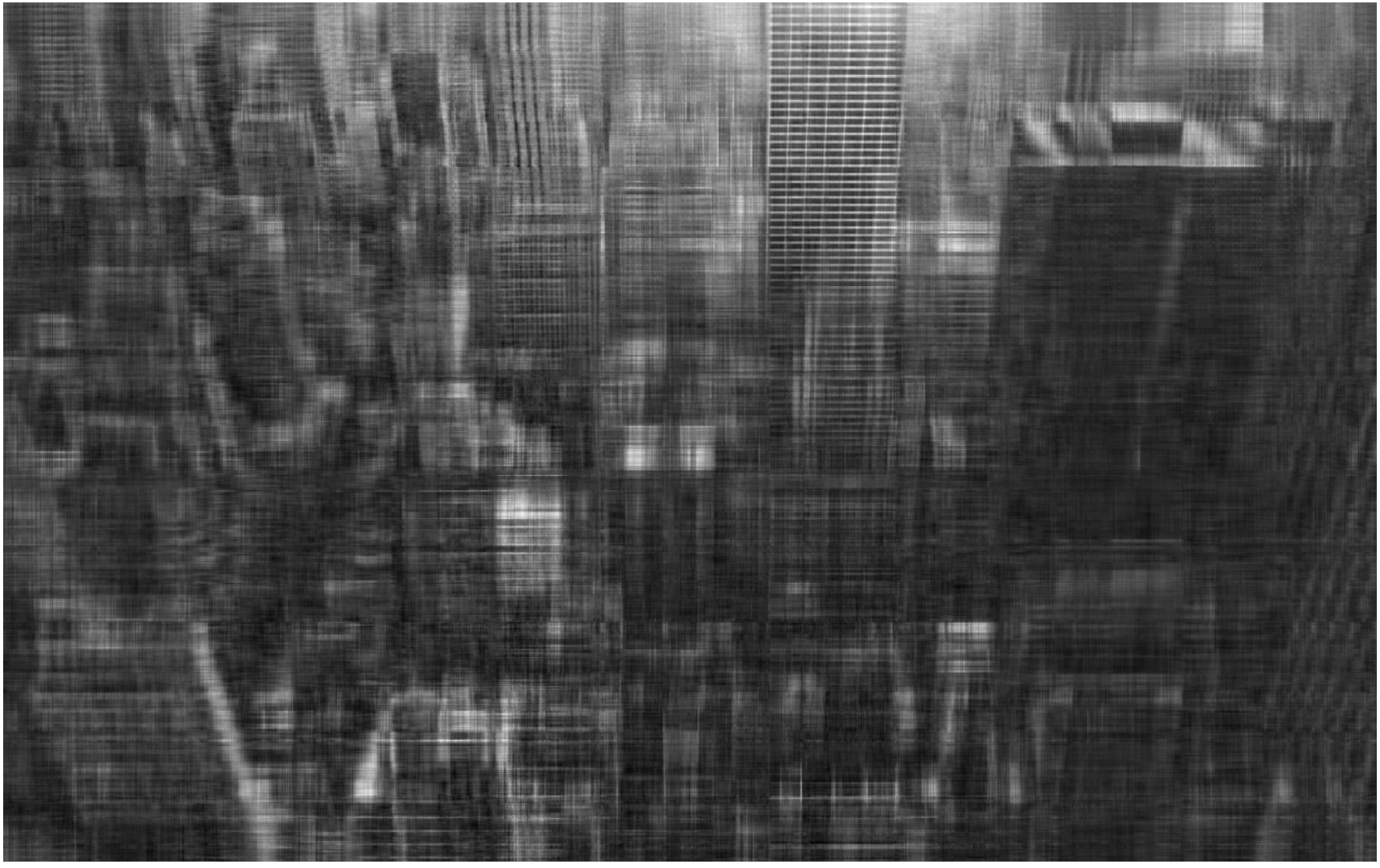

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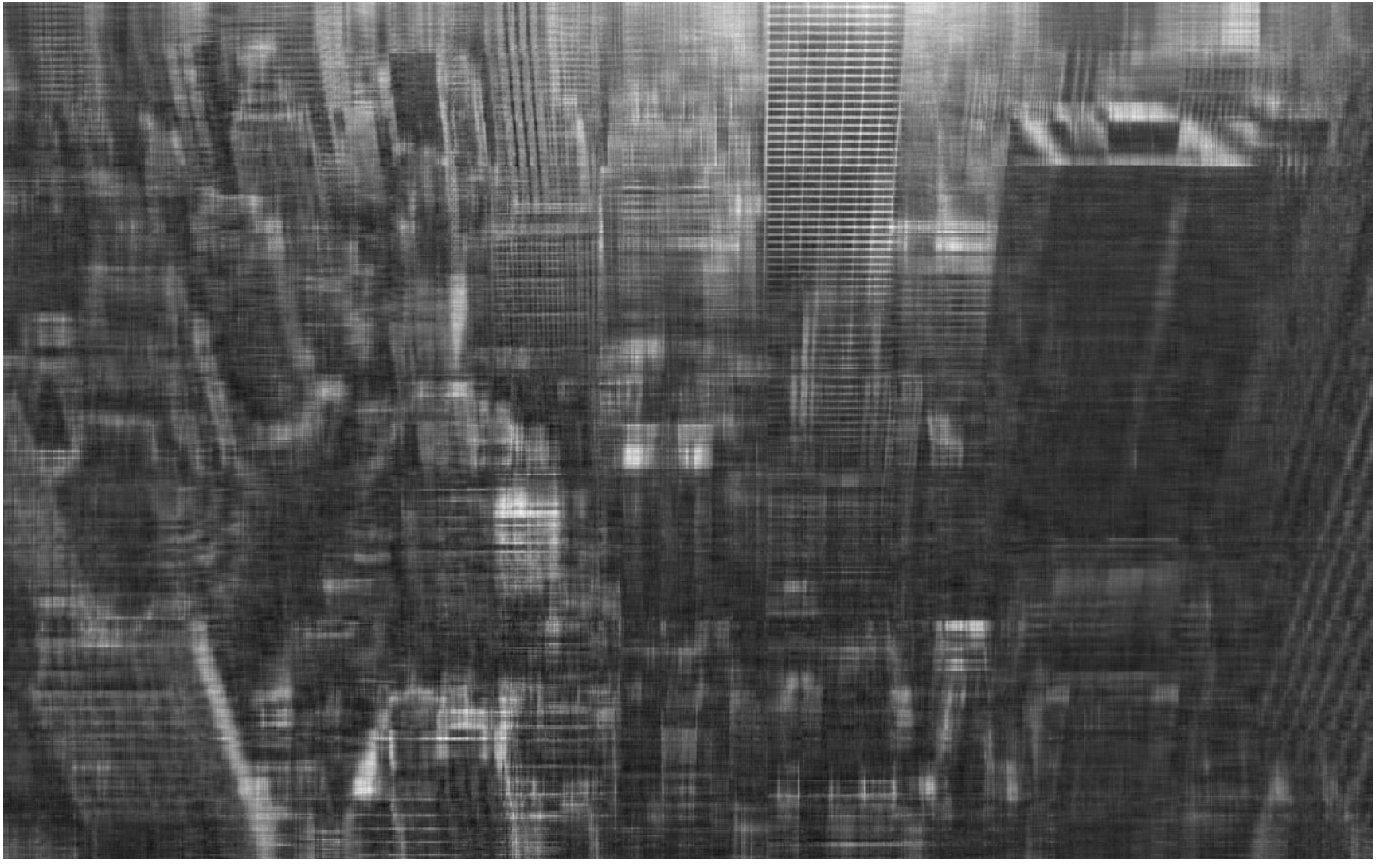

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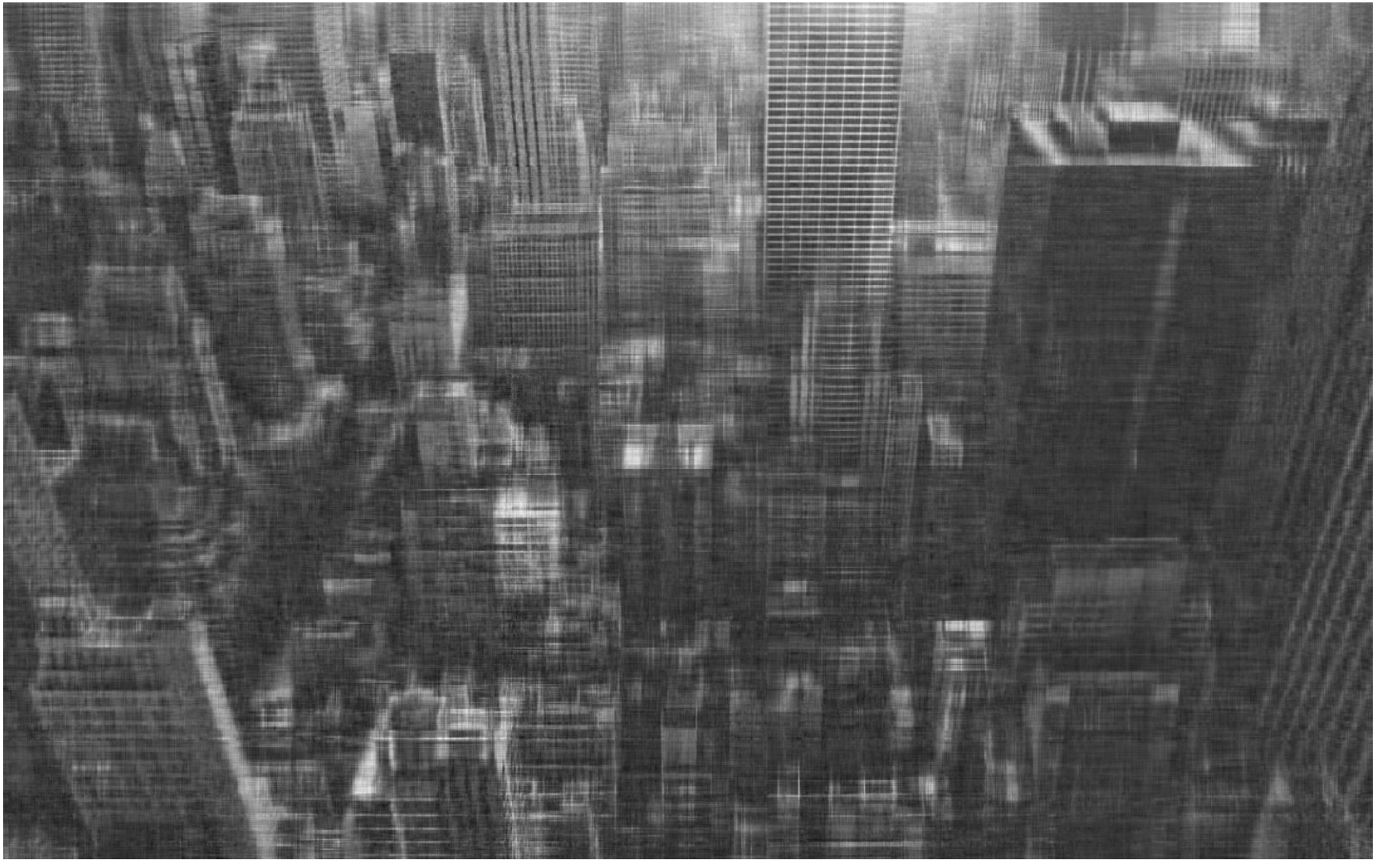

Collaborative Filtering, Matrix Completion

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Collaborative Filtering, Matrix Completion

Exact reconstruction (no noise)

$$\hat{R} \in \operatorname{argmin}\{\|M\|_* \text{ such that } \mathcal{P}_E(M) = \mathcal{P}_E(R)\}$$

Assume $n = n_U = n_I$ for short and put $m = |E|$. Then under some assumptions

- No method can suceed if $m \leq crn \log n$. Namely, need **at least**

  $$m \geq crn \log n$$

  observed entries to recover M and $r = \text{rank}$
- If $m \geq crn(\log n)^2$ then reconstruction is **exact**! with a large probability
- In this setting, convex relaxation is **exact**: **no loss** when relaxing rank by $\|\cdot\|_*$
- Gives the exact same solution as the one constrained by rank!
- Convex programming incredibly powerful in this case
- Compressed sensing theory

Thank you!