Randomness in reduced order modeling

Akil Narayan¹

¹Department of Mathematics, and Scientific Computing and Imaging (SCI) Institute University of Utah

> February 7, 2020 ICERM





Many things that are difficult to accomplish with deterministic optimization/algorithms can be accomplished* with randomization.

Many things that are difficult to accomplish with deterministic optimization/algorithms can be accomplished* with randomization.

*: with "high" probability

Randomness is your friend

Many things that are difficult to accomplish with deterministic optimization/algorithms can be accomplished* with randomization.

*: with "high" probability

We'll consider three examples of this in ROM:

- RBM for elliptic PDE's
- Sparse approximation
- Measure atomization/discretization

Randomness is your friend

Many things that are difficult to accomplish with deterministic optimization/algorithms can be accomplished* with randomization.

*: with "high" probability

We'll consider three examples of this in ROM:

- RBM for elliptic PDE's
- Sparse approximation
- Measure atomization/discretization

Why is randomness helpful?

Intuition is straightforward and simplistic: Let X be a random variable.

Let $(X_m)_{m \ge 1}$ be iid copies of X. Law of large numbers:

$$S \coloneqq \sum_{m=1}^{M} X_m \to \mathbb{E}[X].$$

Why is randomness helpful?

Intuition is straightforward and simplistic: Let X be a random variable.

Let $(X_m)_{m \ge 1}$ be iid copies of X. Law of large numbers:

$$S \coloneqq \sum_{m=1}^{M} X_m \to \mathbb{E}[X].$$

Furthermore, this convergence is quantitative through the Central limit theorem:

$$S(M) - \mathbb{E}[X] \sim \mathcal{N}\left(0, \frac{\sigma^2(X)}{M}\right).$$

In other words, S concentrates around $\mathbb{E}[X]$.

Why is randomness helpful?

Intuition is straightforward and simplistic: Let X be a random variable.

Let $(X_m)_{m \ge 1}$ be iid copies of X. Law of large numbers:

$$S \coloneqq \sum_{m=1}^{M} X_m \to \mathbb{E}[X].$$

Furthermore, this convergence is quantitative through the Central limit theorem:

$$S(M) - \mathbb{E}[X] \sim \mathcal{N}\left(0, \frac{\sigma^2(X)}{M}\right).$$

In other words, S concentrates around $\mathbb{E}[X]$.

This statement is quite powerful:

- S provides an estimator for $\mathbb{E}[X]$, without knowing $\mathbb{E}[X]$.
- Convergence is essentially *independent* of distribution of X.
- Convergence rate is *independent* of *dimension* of *X*.

Concentration in general plays an important role in computing estimates:

- Monte Carlo (CLT) estimates
- Chebyshev inequalities (bounds on mass away from the mean)
- Hoeffding inequalities (bounds on deviation of iid sums from the mean)
- Chernoff bounds (bounds on deviation of spectrum)
- Concentration of measure (bounds on deviation of random functions)

Today: We'll see a particular Chernoff bound in action.

Chernoff bound applications

We will see how randomization and Chernoff bounds can be applied to:

- RBM for elliptic PDE's
- Sparse approximation
- Measure atomization/discretization

Before discussing ROM, let's present the Chernoff bound.

Matrix law of large numbers

Let $\pmb{G} \in \mathbb{R}^{N \times N}$ be a Gramian matrix that is an iid sum of symmetric rank-1 matrices.

I.e., let $\boldsymbol{X} \in \mathbb{R}^N$ have distribution μ on \mathbb{R}^N , and define

$$\boldsymbol{G} \coloneqq \frac{1}{M} \sum_{m=1}^{M} \boldsymbol{X}_m \boldsymbol{X}_m^T,$$

where $\{X_m\}_{m \ge 1}$ are iid copies of X.

Chernoff bounds make quantitative statements about the spectrum of G that depend on the distribution of X.

Matrix law of large numbers

Let $\boldsymbol{G} \in \mathbb{R}^{N \times N}$ be a Gramian matrix that is an iid sum of symmetric rank-1 matrices.

I.e., let $\boldsymbol{X} \in \mathbb{R}^N$ have distribution μ on \mathbb{R}^N , and define

$$\boldsymbol{G} \coloneqq \frac{1}{M} \sum_{m=1}^{M} \boldsymbol{X}_m \boldsymbol{X}_m^T,$$

where $\{X_m\}_{m \ge 1}$ are iid copies of X.

Chernoff bounds make quantitative statements about the spectrum of G that depend on the distribution of X.

For large M, we expect that

$$(G)_{j,k} \xrightarrow{M \uparrow \infty} \mathbb{E}[X_j X_k].$$

Matrix law of large numbers

Let $\boldsymbol{G} \in \mathbb{R}^{N \times N}$ be a Gramian matrix that is an iid sum of symmetric rank-1 matrices.

I.e., let $\boldsymbol{X} \in \mathbb{R}^N$ have distribution μ on \mathbb{R}^N , and define

$$\boldsymbol{G} \coloneqq \frac{1}{M} \sum_{m=1}^{M} \boldsymbol{X}_m \boldsymbol{X}_m^T,$$

where $\{X_m\}_{m \ge 1}$ are iid copies of X.

Chernoff bounds make quantitative statements about the spectrum of G that depend on the distribution of X.

For large M, we expect that

$$(G)_{j,k} \xrightarrow{M \uparrow \infty} \mathbb{E}[X_j X_k].$$

For simplicity, in all that follows we assume that the components of \boldsymbol{X} are

- uncorrelated,
- of unit variance,

so that

$$G \stackrel{M \uparrow \infty}{\longrightarrow} I$$

Matrix Chernoff bounds

The proximity of G to I, as a function of M, is determined by

$$K \coloneqq \sup_{\boldsymbol{X}} \|\boldsymbol{X}\|_2,$$

which is assumed finite.

Matrix Chernoff bounds

The proximity of G to I, as a function of M, is determined by

$$K \coloneqq \sup_{\boldsymbol{X}} \|\boldsymbol{X}\|_2,$$

which is assumed finite.

Theorem ([Cohen, Davenport, Leviatan 2012]) Assume that

$$\frac{M}{\log M} \gtrsim \frac{K}{\delta^2} \log\left(\frac{1}{\epsilon}\right).$$

Then,

$$\Pr\left[(\sigma_{\min}(\boldsymbol{G}) < 1 - \delta) \bigcup (\sigma_{\max}(\boldsymbol{G}) > 1 + \delta)\right] \leq \epsilon.$$

Matrix Chernoff bounds

The proximity of G to I, as a function of M, is determined by

$$K \coloneqq \sup_{\boldsymbol{X}} \|\boldsymbol{X}\|_2,$$

which is assumed finite.

Theorem ([Cohen, Davenport, Leviatan 2012]) Assume that

$$\frac{M}{\log M} \gtrsim \frac{K}{\delta^2} \log\left(\frac{1}{\epsilon}\right).$$

Then,

$$\Pr\left[(\sigma_{\min}(\boldsymbol{G}) < 1 - \delta) \bigcup (\sigma_{\max}(\boldsymbol{G}) > 1 + \delta)\right] \leq \epsilon.$$

What can we do with G? Form least-squares approximations using X. Remarks:

- The δ^{-2} dependence is "CLT-like".
- K is the only thing that depends on the distribution of X.

It turns out that K can be quite large (or infinite) for practical situations.

A fix for this utilizes importance sampling. In particular, define

$$\mathrm{d}\rho(x) \coloneqq \left(\frac{1}{N}\sum_{n=1}^N x_n^2\right)\mathrm{d}\mu(x),$$

where μ is the distribution of X.

 ρ is a probability measure on \mathbb{R}^N , and is frequently called the *induced distribution*.

A (more) optimal Chernoff bound

In practical scenarios, the induced distribution ρ can also be sampled from without too much effort.

More importantly, we can get a (much) better Chernoff bound here.

Let $(\mathbf{Y}_m)_{m \ge 1} \in \mathbb{R}^N$ be iid samples from ρ . We need to weight the Gramian so that we produce an unbiased estimate:

$$\boldsymbol{F} \coloneqq \frac{1}{M} \sum_{m=1}^{M} w_m \boldsymbol{Y}_m \boldsymbol{Y}_m^T, \qquad \qquad w_m \coloneqq \frac{\mathrm{d}\mu}{\mathrm{d}\rho} (\boldsymbol{Y}_m)$$

A (more) optimal Chernoff bound

In practical scenarios, the induced distribution ρ can also be sampled from without too much effort.

More importantly, we can get a (much) better Chernoff bound here.

Let $(\mathbf{Y}_m)_{m \ge 1} \in \mathbb{R}^N$ be iid samples from ρ . We need to weight the Gramian so that we produce an unbiased estimate:

$$\boldsymbol{F} \coloneqq \frac{1}{M} \sum_{m=1}^{M} w_m \boldsymbol{Y}_m \boldsymbol{Y}_m^T, \qquad \qquad w_m \coloneqq \frac{\mathrm{d}\mu}{\mathrm{d}\rho} (\boldsymbol{Y}_m)$$

This results in the (better) Chernoff bound

$$\Pr\left[(\sigma_{\min}(\boldsymbol{F}) < 1 - \delta) \bigcup (\sigma_{\min}(\boldsymbol{F}) > 1 + \delta)\right] \leq \epsilon,$$

with the much more reasonable assumption

$$\frac{M}{\log M} \gtrsim \frac{N}{\delta^2} \log\left(\frac{1}{\epsilon}\right).$$

This Chernoff bound will be a seed for achieving model reduction.

Example 1: RBM (for elliptic problems)

Reduced basis methods

For the parameterized problem,

$$-\nabla \cdot \left(\sum_{j=1}^{\infty} \mu_j a_j(x) \nabla u\right) = b,$$

with $\mu \in [-1,1]^\infty$, recall that RBM (essentially) iteratively computes

$$\arg\max_{\mu} \left\| u(\mu) - \mathcal{P}_{j-1}(u(\mu)) \right\|,$$

Reduced basis methods

For the parameterized problem,

$$-\nabla \cdot \left(\sum_{j=1}^{\infty} \mu_j a_j(x) \nabla u\right) = b,$$

with $\mu \in [-1,1]^{\infty}$, recall that RBM (essentially) iteratively computes

$$\arg\max_{\mu} \left\| u(\mu) - \mathcal{P}_{j-1}(u(\mu)) \right\|,$$

If (any truncation of) μ is high-dimensional, this is an expensive optimization, even if the objective is easy to evaluate.

There's a bigger problem: the $\arg \max$ is typically taken over a discrete μ grid. If μ is high-dimensional, how can we certify error without densely sampling?

Reduction feasibility

Some analysis gives us a strategy to proceed: if the $\{a_j\}_{j=1}^d$ satisfies an ℓ^p summability condition,

$$\sum_{j=1}^{\infty} \|a_j\|_{L^{\infty}}^p < \infty, \qquad \qquad p < 1,$$

then there is an $N\text{-dimensional}\ downward-closed$ polynomial space P_N in the variable μ such that

$$\sup_{\mu} \left\| u(\mu) - \operatorname{Proj}_{P_N} u(\mu) \right\| \leqslant N^{-s}, \qquad \qquad s \coloneqq \frac{1}{p} - \frac{1}{2}.$$

There are constructive algorithms to essentially identify P_N , [Cohen, Devore, Schwab 2011].

In particular, once P_N is identified, this approximation can be obtained by $\mu\text{-least-squares}$ approximation.

I.e., if we can certify accuracy on a "*polynomial* grid", we can probably obtain accuracy.

Let μ be a random variable with distribution ν .

I.e., if we can certify accuracy on a "*polynomial* grid", we can probably obtain accuracy.

Let μ be a random variable with distribution ν . Let $\mathbf{X} = (X_n(\nu))_{n=1}^N$ denote a $d\nu$ -orthonormal basis for P_N . Define the induced distribution $\rho = \rho(\nu, \mathbf{X})$ based on this, sample $\{\mathbf{Y}_m\}_{m\geq 1}^M$ from ρ , and use this to discretize the $\arg \max$ procedure in RBM.

Let $u_N(\mu)$ denote the resulting N-degree of freedom RBM surrogate.

I.e., if we can certify accuracy on a "*polynomial* grid", we can probably obtain accuracy.

Let μ be a random variable with distribution ν . Let $\mathbf{X} = (X_n(\nu))_{n=1}^N$ denote a $d\nu$ -orthonormal basis for P_N . Define the induced distribution $\rho = \rho(\nu, \mathbf{X})$ based on this, sample $\{\mathbf{Y}_m\}_{m\geq 1}^M$ from ρ , and use this to discretize the $\arg \max$ procedure in RBM.

Let $u_N(\mu)$ denote the resulting N-degree of freedom RBM surrogate.

lf

$$\frac{M}{\log M} \gtrsim \frac{N}{\delta^2} \log\left(\frac{1}{\epsilon}\right),$$

then the least-squares P_N -polynomial approximation $v_N(\mu) \in P_N$ to u_N satisfies

$$\mathbb{E}\left[v_N(\mu) - u(\mu)\right]^2 \lesssim N^{-2s} + U^2 \epsilon \frac{1+\delta}{1-\delta},$$

where U is the uniform bound $U = \sup_{\mu} \|u(\mu)\|$.

I.e., if we can certify accuracy on a "*polynomial* grid", we can probably obtain accuracy.

Let μ be a random variable with distribution ν . Let $\boldsymbol{X} = (X_n(\nu))_{n=1}^N$ denote a $d\nu$ -orthonormal basis for P_N . Define the induced distribution $\rho = \rho(\nu, \boldsymbol{X})$ based on this, sample $\{\boldsymbol{Y}_m\}_{m\geq 1}^M$ from ρ , and use this to discretize the $\arg \max$ procedure in RBM.

Let $u_N(\mu)$ denote the resulting N-degree of freedom RBM surrogate.

lf

$$\frac{M}{\log M} \gtrsim \frac{N}{\delta^2} \log\left(\frac{1}{\epsilon}\right),$$

then the least-squares P_N -polynomial approximation $v_N(\mu) \in P_N$ to u_N satisfies

$$\mathbb{E}\left[v_N(\mu) - u(\mu)\right]^2 \lesssim N^{-2s} + U^2 \epsilon \frac{1+\delta}{1-\delta},$$

where U is the uniform bound $U = \sup_{\mu} ||u(\mu)||$. Without randomization, such a rigorous bound is practically infeasible.

Example 2: Sparse (polynomial) approximation

Underdetermined systems

Let x_0 be a signal (vector) in \mathbb{R}^N . If we have $M \ge N$ linear measurements of x_0 :

$$\boldsymbol{b} \coloneqq \boldsymbol{A} \boldsymbol{x}_0,$$

then there is (usually) a unique solution x^* that minimizes the ℓ^2 discrepancy:

$$\boldsymbol{x}^* \coloneqq \operatorname*{arg\,min}_{\boldsymbol{z} \in \mathbb{R}^N} \|\boldsymbol{A}\boldsymbol{z} - \boldsymbol{b}\|_2.$$

And (usually), $\boldsymbol{x^*} = \boldsymbol{x}_0$.

Underdetermined systems

Let x_0 be a signal (vector) in \mathbb{R}^N . If we have $M \ge N$ linear measurements of x_0 :

$$\boldsymbol{b} \coloneqq \boldsymbol{A} \boldsymbol{x}_0,$$

then there is (usually) a unique solution x^* that minimizes the ℓ^2 discrepancy:

$$\boldsymbol{x}^* \coloneqq \operatorname*{arg\,min}_{\boldsymbol{z} \in \mathbb{R}^N} \|\boldsymbol{A}\boldsymbol{z} - \boldsymbol{b}\|_2.$$

And (usually), $x^* = x_0$. The situation is (far) more complicated if M < N.

This is a particularly salient concern for MOR: x may be a high-dimensional model, but we may only have a small number of measurements.

Compressive sampling

How can we make this problem well-posed?

Suppose that x_0 is *s*-sparse, i.e., the number of non-zero terms is at most $s \ll N$. We can consider the optimization problem,

 $\min \|\boldsymbol{z}\|_0 \quad \text{such that} \quad \boldsymbol{A}\boldsymbol{z} = \boldsymbol{b}.$

This problem is well-posed under mild conditions.

Compressive sampling

How can we make this problem well-posed?

Suppose that x_0 is *s*-sparse, i.e., the number of non-zero terms is at most $s \ll N$. We can consider the optimization problem.

 $\min \|\boldsymbol{z}\|_0 \quad \text{such that} \quad \boldsymbol{A}\boldsymbol{z} = \boldsymbol{b}.$

This problem is well-posed under mild conditions.

Unfortunately, it's also NP-hard. A (fairly naive) relaxation of this problem is

 $\min \|\boldsymbol{z}\|_1$ such that $A\boldsymbol{z} = \boldsymbol{b}$.

This is a *convex* problem, and hence it is computationally practical to solve.

Compressive sampling

How can we make this problem well-posed?

Suppose that x_0 is *s*-sparse, i.e., the number of non-zero terms is at most $s \ll N$. We can consider the optimization problem.

 $\min \|\boldsymbol{z}\|_0 \quad \text{such that} \quad \boldsymbol{A}\boldsymbol{z} = \boldsymbol{b}.$

This problem is well-posed under mild conditions.

Unfortunately, it's also NP-hard. A (fairly naive) relaxation of this problem is

 $\min \|\boldsymbol{z}\|_1$ such that $A\boldsymbol{z} = \boldsymbol{b}$.

This is a *convex* problem, and hence it is computationally practical to solve.

If x_0 is sparse, does the ℓ^1 minimization problem recover the sparse solution?

Null space and restricted isometry properties

The matrix A satisfies the (robust) *null space property* (NSP) with constant c and sparsity s if

$$\|\boldsymbol{k}_S\|_1 \leqslant c \, \|\boldsymbol{k}_{S^c}\|_1 \,, \tag{1}$$

holds for every $k \in \text{ker}(A)$, and every subset $S \subset [N]$ with cardinality at most s.

Needless to say this is a rather difficult condition to verify directly.

But: (1) is a necessary and sufficient condition so that ℓ^1 minimization and ℓ^0 minimization are equivalent. [Cohen, Devore 2009]

Null space and restricted isometry properties

The matrix A satisfies the (robust) *null space property* (NSP) with constant c and sparsity s if

$$\|\boldsymbol{k}_S\|_1 \leqslant c \, \|\boldsymbol{k}_{S^c}\|_1 \,, \tag{1}$$

holds for every $k \in \text{ker}(A)$, and every subset $S \subset [N]$ with cardinality at most s.

Needless to say this is a rather difficult condition to verify directly.

But: (1) is a necessary and sufficient condition so that ℓ^1 minimization and ℓ^0 minimization are equivalent. [Cohen, Devore 2009]

There is a stronger condition to ensure that ℓ^1 minimization can compute sparse solutions, the *restricted isometry property* (RIP).

 $oldsymbol{A}$ satisfies the RIP with constant ϵ and sparsity s if

$$(1-\epsilon) \|\boldsymbol{x}\|_2 \leq \|\boldsymbol{A}\boldsymbol{x}\|_2 \leq (1+\epsilon) \|\boldsymbol{x}\|_2,$$

for every s-sparse vector \boldsymbol{x} .

This condition may also seem difficult to verify, but it contains ℓ^2 norms!

The virtue of the RIP is that:

$$RIP \Longrightarrow NSP(\iff \ell^1 \equiv \ell^0)$$

and the RIP is much easier to verify. [Candes, Tao 2005]

The virtue of the RIP is that:

$$RIP \Longrightarrow NSP(\Longleftrightarrow \ell^1 \equiv \ell^0)$$

and the RIP is much easier to verify. [Candes, Tao 2005]

In particular, suppose that $\boldsymbol{B} \in \mathbb{R}^{P \times N}$ with $P \ge N$ satisfies

$$1 - \delta \leq \sigma_{\min}(\boldsymbol{B}), \qquad \sigma_{\max}(\boldsymbol{B}) \leq 1 + \delta.$$

Now, form A from B by uniformly at random subsampling M rows from B.

The virtue of the RIP is that:

$$\mathrm{RIP} \Longrightarrow \mathrm{NSP}(\Longleftrightarrow \ell^1 \equiv \ell^0)$$

and the RIP is much easier to verify. [Candes, Tao 2005]

In particular, suppose that $\boldsymbol{B} \in \mathbb{R}^{P \times N}$ with $P \ge N$ satisfies

$$1 - \delta \leq \sigma_{\min}(\boldsymbol{B}), \qquad \sigma_{\max}(\boldsymbol{B}) \leq 1 + \delta.$$

Now, form A from B by uniformly at random subsampling M rows from B. Then A satisfies the (s,ϵ) RIP "with high probability" if

$$M \gtrsim K \log\left(\frac{1}{\epsilon}\right) \frac{1}{1-\delta^2} s \log^3(s) \log N,$$

where K is the maximum row norm of B.[Rauhut 2010]

The virtue of the RIP is that:

$$\mathrm{RIP} \Longrightarrow \mathrm{NSP}(\Longleftrightarrow \ell^1 \equiv \ell^0)$$

and the RIP is much easier to verify. [Candes, Tao 2005]

In particular, suppose that $\boldsymbol{B} \in \mathbb{R}^{P \times N}$ with $P \ge N$ satisfies

$$1 - \delta \leq \sigma_{\min}(\boldsymbol{B}), \qquad \sigma_{\max}(\boldsymbol{B}) \leq 1 + \delta.$$

Now, form \boldsymbol{A} from \boldsymbol{B} by uniformly at random subsampling M rows from \boldsymbol{B} .

Then \boldsymbol{A} satisfies the (s,ϵ) RIP "with high probability" if

$$M \gtrsim K \log\left(\frac{1}{\epsilon}\right) \frac{1}{1-\delta^2} s \log^3(s) \log N,$$

where K is the maximum row norm of B.[Rauhut 2010]

The problems: (i) K can be very large, and (ii) sometimes P must be (extremely) large before δ is small.

The major point

If ${\boldsymbol{B}}$ is a matrix with "nearly" orthonormal columns, and maximum row norm K, then forming ${\boldsymbol{A}}$ with

$$M \sim Ks$$

subsampled rows yields an RIP matrix.

Hence, if b contains measurements from a sparse vector x_0 , then (with high probability) the solution to

$$\min \|\boldsymbol{z}\|_1 \quad \text{such that} \quad \boldsymbol{A}\boldsymbol{z} = \boldsymbol{b},$$

is the sparse vector x_0 .

The major point (optimized)

From the Chernoff bound: Forming \boldsymbol{A} with

 $M \sim \mathbf{1}s$

subsampled rows yields an RIP matrix, if:

- we form \boldsymbol{B} by taking $P \sim N \log N$ samples from the induced distribution
- we use the appropriate biasing weights to rescale A.

Hence with $M \sim s$ samples, we can guarantee recovery of sparse vectors with sparse measurements.[Adcock, Brugiapaglia, Razi, N 2020]

The major point (optimized)

From the Chernoff bound: Forming \boldsymbol{A} with

 $M \sim 1s$

subsampled rows yields an RIP matrix, if:

- we form \boldsymbol{B} by taking $P \sim N \log N$ samples from the induced distribution
- we use the appropriate biasing weights to rescale A.

Hence with $M \sim s$ samples, we can guarantee recovery of sparse vectors with sparse measurements.[Adcock, Brugiapaglia, Razi, N 2020]

This type of guarantee is $\underbrace{\mathsf{extremely}}_{randomization.}$ difficult to achieve in general without

Randomness is your friend

Many things that cannot be accomplished with deterministic methods can be accomplished * with randomization.

*: with "high" probability

We looked at two examples of this in ROM:

- RBM for elliptic PDE's
- Sparse approximation

There are *many* more examples.