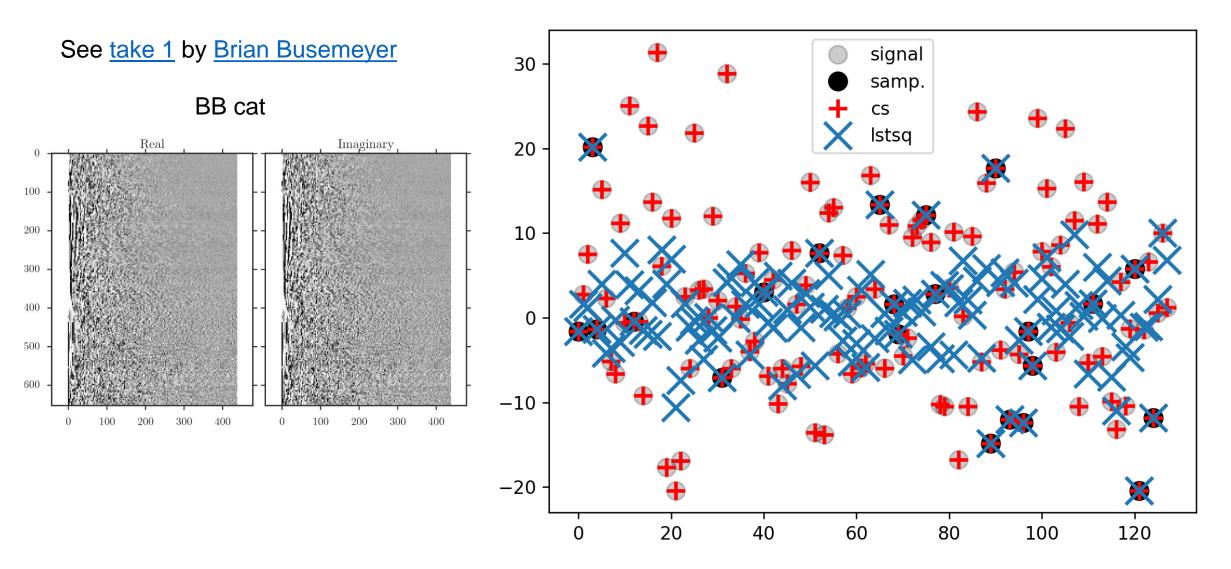
Compressive Sensing Take 2

Yubo "Paul" Yang, Algorithm Interest Group, Nov. 1 2019



What is compressive (compressed) sensing?

Compressive sensing is a signal processing technique to reconstruct sparse signal from few samples.

It solves a system of underdetermined linear equations by imposing sparsity as a constraint.

solve y = A x when len(y) \ll len(x) by minimizing the number of non-zero entries in x.



Trick: x has to be sparse.

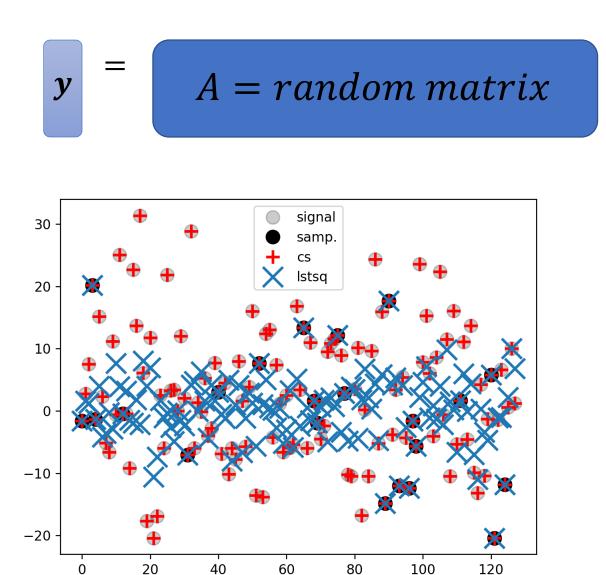
Simplest example: random transform of a very sparse sample

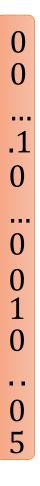
Goal: use y with a small length to recover x

Strategy: minimize the L1-norm of x

nfull = 128parse signal x = np.zeros(nfull)x[1] = 1x[42] = 10x[101] = .5signal in dense space pp.random.seed(1836) amat 🕨 np.random.randn(nfull, nfull) y = np.dot(x, amat) sample signal in dense space nsamp = 22idx = np.arange(nfull) isamp = np.random.choice(idx, nsamp, ysamp = y[isamp] asamp = amat[:, isamp]

xarr = cs(asamp, ysamp) xl2 = np.linalg.lstsq(asamp.T, ysamp)[0]



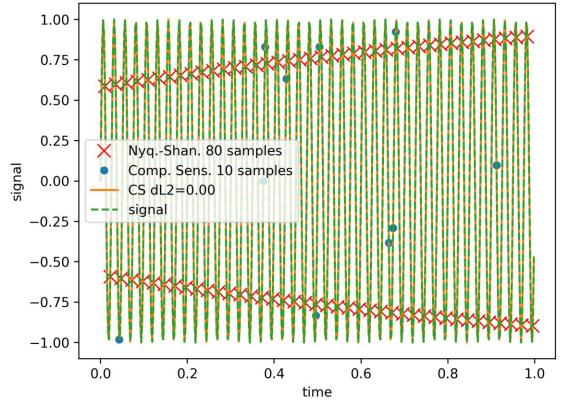


Practical application I: digital to analog conversion below Nyquist-Shannon

In practice, constructing the A matrix can be tricky.

Signal in time domain, use Fourier transform as A matrix.

```
# build FFT basis transformation matrix
amat = []
for irow in range(nfull):
   vec = np.zeros(nfull, dtype=complex)
   vec[irow] = 1
   row = np.fft.ifft(vec)
   amat.append(row)
amat = np.array(amat)
```

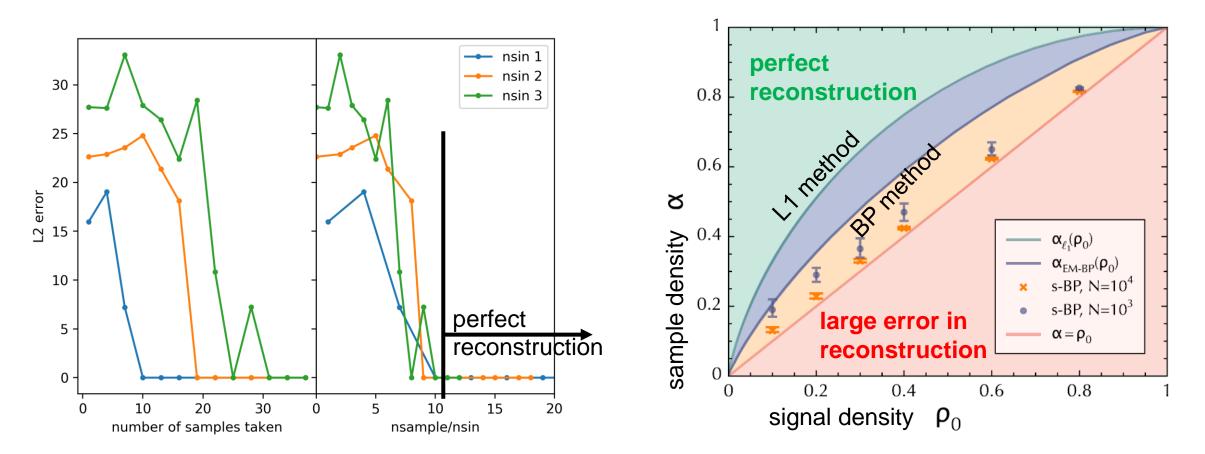


How many samples does it take?

Toy problem: reconstruct a sum of sine waves

$$y(t) = \sum_{n=1}^{n \sin n} \sin(2\pi n t)$$

Number of samples needed for perfect reconstruction is determined by signal sparsity in "good" basis.



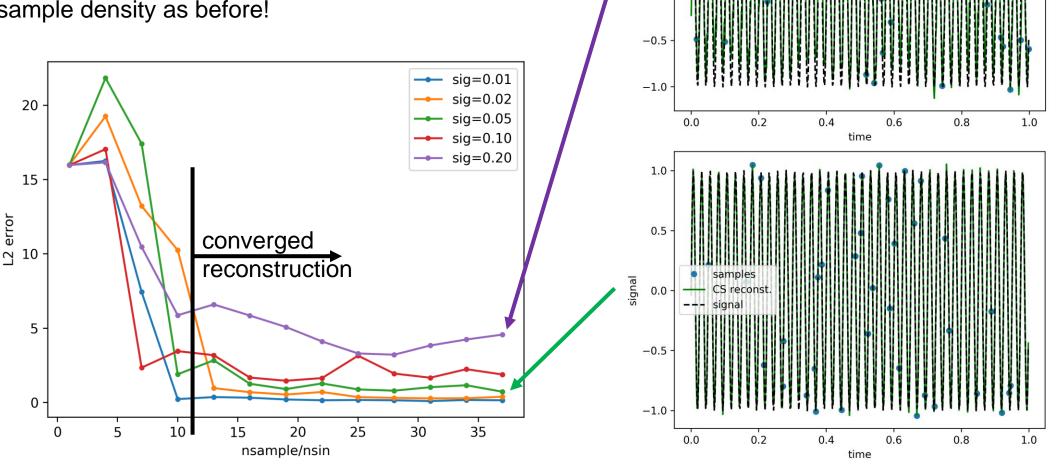
F. Krzakala, M. Mezard, F. Sausset, Y.F. Sun, and L. Zdeborova, Phys. Rev. X 2, 021005 (2012).

How robust is CS to noise?

Reconstruction is robust up to 5% white noise.

Reconstruction noise does increase with more noise.

but error converges roughly at the same transition sample density as before!



1.5

1.0

0.5

0.0

CS recons

signal

signal

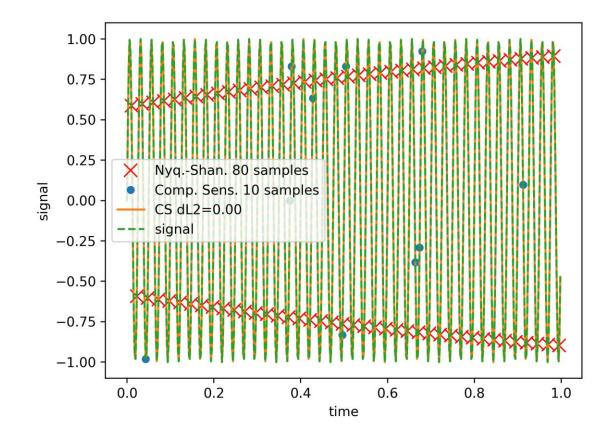
Why is compressive sensing useful?

Signal reconstruction while under-sampling (lower average freq. than Nyquist-Shannon)

Image reconstruction single-pixel camera fast MRI

Digital to analog conversion

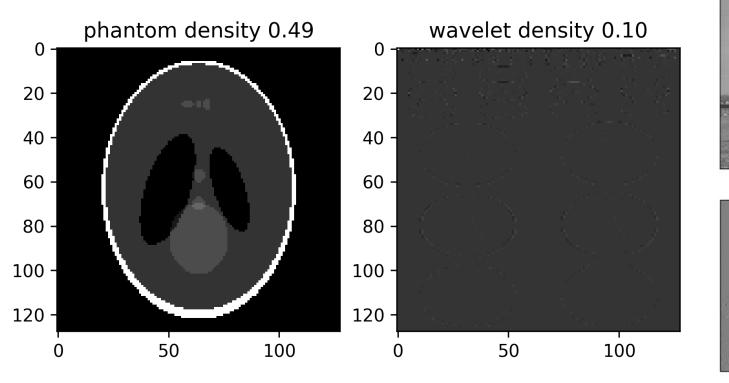
Map Born-Oppenheimer potential energy surface using phonon directions!



Practical application II: image compression

In the spirit of Halloween, let us attempt a reconstruction of the Shepp-Logan phantom.

2D images, use wavelet transform as A matrix.



pywt package provides forward and inverse transforms

Approximation

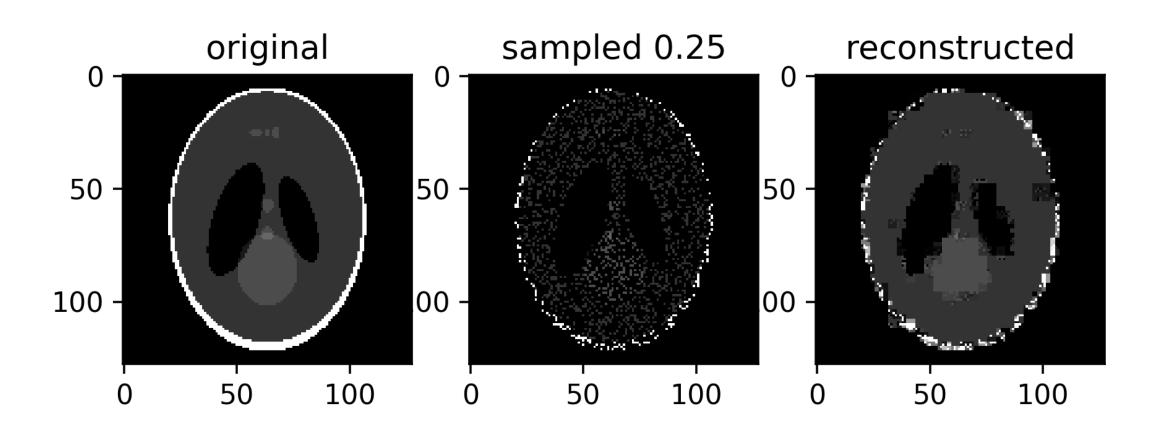
Vertical detail

Horizontal detail

Diagonal detail

Practical application II: image compression

My attempt: spooky?



Application to Physics I: MD vibrational spectrum

Accurate frequency after a few MD time steps

velocity-velocity correlation

$$\gamma(t) = \frac{\left\langle \sum_{i} \mathbf{v}_{i}(t) \cdot \mathbf{v}_{i}(0) \right\rangle}{\left\langle \sum_{i} \mathbf{v}_{i}(0) \cdot \mathbf{v}_{i}(0) \right\rangle},$$
$$f(\omega) = \int dt \gamma(t) \cos(\omega t).$$

is sparse in Fourier space

Same problem as our practical application I

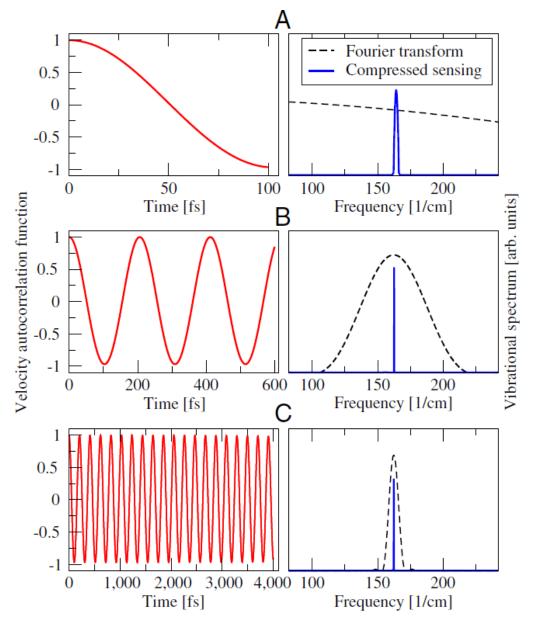


Fig. 1. Frequency distribution spectrum of Na₂ calculated using FT and CS for different total propagation times: (A) 100 fs, (B) 600 fs, and (C) 4,000 fs.

X. Andrade, J. N. Sanders, and A. Aspuru-Guzik, Proc. Natl. Acad. Sci. U. S. A. 109, 13928-13933 (2012).

Application to Physics II: Lattice dynamics

 $V = V_0 + \Phi_{\mathbf{a}} u_{\mathbf{a}} + \frac{\Phi_{\mathbf{abc}}}{2} u_{\mathbf{a}} u_{\mathbf{b}} + \frac{\Phi_{\mathbf{abc}}}{3!} u_{\mathbf{a}} u_{\mathbf{b}} u_{\mathbf{c}} + \cdots, \quad (1) \text{ force-displacement relationship for Eq. (1),}$

where $u_{\mathbf{a}} \equiv u_{a,i}$ is the displacement of atom *a* at a lattice site \mathbf{R}_a in the Cartesian direction *i*, the second-order expansion coefficients $\Phi_{\mathbf{ab}} \equiv \Phi_{ij}(ab) = \partial^2 V / \partial u_{\mathbf{a}} \partial u_{\mathbf{b}}$ determine the phonon dispersion in the harmonic approximation, and $\Phi_{\mathbf{abc}} \equiv \Phi_{ijk}(abc) = \partial^3 V / \partial u_{\mathbf{a}} \partial u_{\mathbf{b}} \partial u_{\mathbf{c}}$, etc., are third- and higher-order anharmonic force constant tensors (FCTs). The linear term with $\Phi_{\mathbf{a}}$ is absent if the

$$F_{\mathbf{a}} = -\Phi_{\mathbf{a}} - \Phi_{\mathbf{a}\mathbf{b}} u_{\mathbf{b}} - \Phi_{\mathbf{a}\mathbf{b}\mathbf{c}} u_{\mathbf{b}} u_{\mathbf{c}}/2 - \cdots.$$
(2)

The forces can be obtained from first-principles calculations using any general-purpose DFT code for a set of Latomic configurations in a supercell. This establishes a linear problem $\mathbf{F} = \mathbb{A}\Phi$ for the unknown FCTs, where

$$A = \begin{bmatrix} -1 & -u_{\mathbf{b}}^{1} & -\frac{1}{2}u_{\mathbf{b}}^{1}u_{\mathbf{c}}^{1} & \cdots \\ & \cdots & & \\ -1 & -u_{\mathbf{b}}^{L} & -\frac{1}{2}u_{\mathbf{b}}^{L}u_{\mathbf{c}}^{L} & \cdots \end{bmatrix}$$
(3)

will be referred to as the sensing matrix. Its elements are

F. Zhou, W. Nielson, Y. Xia, V. Ozolins, Phys. Rev. Lett. **113**, 18501 (2014).

Application to Physics II: Lattice dynamics

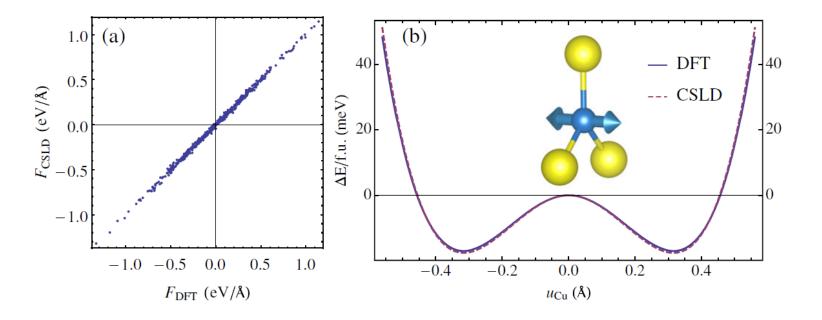
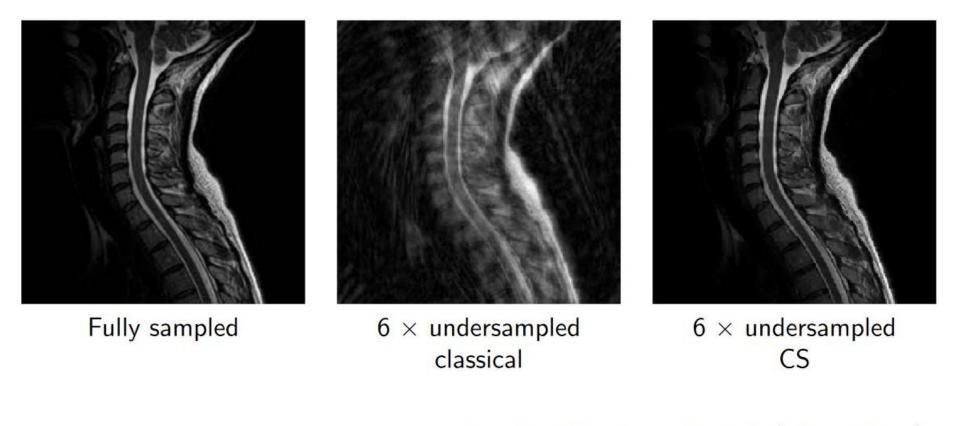


FIG. 3 (color online). Comparison of CSLD predictions with DFT data for tetrahedrite: (a) force at 300 K, (b) relative energy per formula unit of an unstable optical mode involving out-of-plane displacements of trigonally coordinated copper atoms (blue) bonded to sulfur (yellow sphere). DFT and CSLD are shown as solid and dashed lines, respectively.

F. Zhou, W. Nielson, Y. Xia, V. Ozolins, Phys. Rev. Lett. 113, 18501 (2014).

Application to medical imaging: fast MRI



Trzasko, Manduca, Borisch (Mayo Clinic)

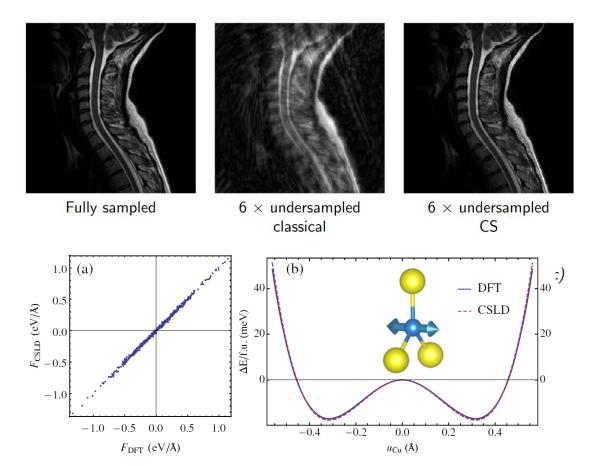
E. Candes, "Compressive Sensing – A 25 Minute Tour," Frontiers of Engineering Symposium, Cambridge, UK (2010).

Conclusions

Compressive sensing is a powerful method for signal reconstruction.

Works whenever your problem is connected to a sparse representation by a linear transform.

It has already found many applications in many fields!



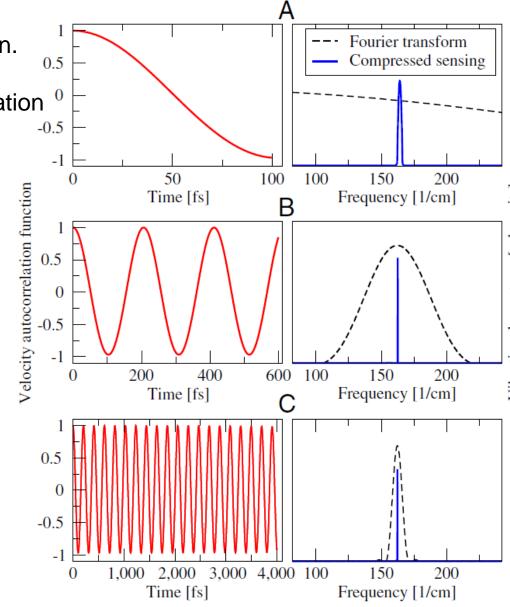


Fig. 1. Frequency distribution spectrum of Na_2 calculated using FT an CS for different total propagation times: (A) 100 fs, (B) 600 fs, and (C) 4,000 fs