Example_StateSpaceViz

January 30, 2025

1 Variance-bounded state-space visualization

1.1 Getting started

If you're not familiar with `python`, I'd start by downloading and installing `anaconda` from https://www.anaconda.com/. Then open up the terminal and create a new `conda` environment: this will give you a playground to install packages in and make sure everything is nice and easy. To do this, use the command

```
conda create --name spring2025
```

or you can call it whatever you like. Then activate the environment with

```
conda activate spring2025
```

I like using `pip` to install software so install `pip` first:

```
conda install pip
```

Then install our libraries:

```
pip install numpy scipy jax matplotlib jupyter ipympl
```

We'll use `numpy` for linear algebra, `scipy` for optimization and more, `jax` for just-in-time compiling and taking derivatives of functions in order to optimize efficiently, `matplotlib` to visualize things, `jupyter` so we can use notebooks such as this one, and finally `ipympl` so we can have interactive matplotlib widgets in notebooks.

Finally, navigate in the terminal to the directory in which you've saved this file, and run

```
jupyter notebook
```

A browser window should open up and you should see this document!

[2]:
```
import numpy as np
import scipy as sc
from scipy.spatial import ConvexHull

import jax
import jax.numpy as jp
from jax import config
config.update("jax_enable_x64", True)

import matplotlib.pyplot as plt
```

```
np.set_printoptions(precision=3, suppress=True)
```

1.2 Generating $P(E_i|\sigma_j)$

As explained in my *Spring 2025 Research Questions*, the theories we'll be investigated depend upon a special conditional probability matrix P which must satisfy some basic constraints. So first off, we're going to have to find a way of randomly generating suitable P's in order to play around with them.

A good P matrix is defined by three parameters:

1. n: $P \in \mathbb{R}^{n\times n}$. Ultimately, the number of reference outcomes.
2. r: the rank of P.
3. α: inverse depolarizing parameter.

As explained in the notes, in terms of these paramters, we can define 1. $\beta = \frac{1-\alpha}{n}$. 2. The Born matrix $\Phi = \alpha I + \beta J$, where J is the matrix of all 1's. 2. $\gamma = \frac{n}{1+\alpha^{-1}(r-1)}$.

We require of P: 1. $\forall i, j : P_{ij} \geq 0$ (non-negativity). 2. $\sum_i P_{ij} = \sum_j P_{ij} = 1$ (bistochastic). 3. $P = P^T$: (symmetric). 4. $\forall i : P(E_i|\sigma_i) = \gamma^{-1}$ (fixed-diagonal). 5. $P\Phi P = P$ (1-inverse).

So how are we going to implement these constraints?

Since P ought to be symmetric, we can write it in terms of a spectral decomposition $P = \sum_{i=0}^{n-1} \lambda_i v_i v_i^T$ where $\{\lambda_i\}, \{v_i\}$ are the eigenvalues and eigenvectors of P respectively. Note: to make things easy to import into python we index from 0. Let $u = (1, \dots, 1)^T$ be the column vector of all 1's. Since P must be bistochastic, u must be an eigenvector with eigenvalue 1. In fact, we should normalize it so it has length 1: $\frac{1}{\sqrt{n}}u$. Now we know from the notes that if P is rank-r, the next $r-1$ eigenvectors must have eigenvalue α^{-1}, and the remaining (which we don't have to worry about) have eigenvalue 0. These eigenvectors must all be orthogonal to each other.

How can we efficiently represent this? Let $O \in \mathbb{R}^{n\times r}$ be the matrix whose columns are the eigenvectors with non-zero eigenvalues of P. We assume the first column is $\frac{1}{\sqrt{n}}u$. Let $D \in \mathbb{R}^{r\times r}$ be the diagonal matrix whose diagonal has a single 1 followed by α^{-1} repeated $r-1$ times. Then we can equivalently write \$ P = O D O^T \$. Demanding orthogonality means that we require $O^T O = I$. If we further demand that $\forall i, j : P_{ij} \geq 0$, then we have a rank-$r$ symmetric, bistochastic matrix which because of its eigenstructure will satisfy $P\Phi P = P$.

But we also need the elements along the diagonal of P to be constant. To analyze this constraint, let's re-write our spectral decomposition

$$P = \frac{1}{n}uu^T + \alpha^{-1}\sum_{i=1}^{r-1} v_i v_i^T.$$

Denoting the k'th basis vector e_k, the diagonal elements are

$$e_k^T P e_k = \frac{1}{n} e_k^T u u^T e_k + \alpha^{-1} \sum_{i=1}^{r-1} e_k^T v_i v_i^T e_k = \frac{1}{n} + \alpha^{-1}\sum_{i=1}^{r-1} O_{ki}^2.$$

If we demand this is equal to γ^{-1}, we have $\frac{1+\alpha^{-1}(r-1)}{n} = \frac{1}{n} + \alpha^{-1}\sum_{i=1}^{r-1} O_{ki}^2$, or

$$\forall k : \sum_{i=1}^{r-1} O_{ki}^2 = \frac{r-1}{n}.$$

In other words, the norms of the vectors formed from the rows O, where we drop the first index, must be fixed.

The following code defines these three constraints and uses `scipy.optimize.minimize` to implement them.

[22]:
```python
n, r, alpha = 4, 3, 3

beta = (1-alpha)/n
gamma = n/(1 + (r-1)/alpha)

u, J = np.ones(n), np.ones((n,n))
Phi = alpha*np.eye(n) + beta*J
D = np.diag([1] + (r-1)*[1/alpha])

# We're going to minimize the following objective function.
# By construction, we have symmetry, eigenstructure, and at least␣
 ↪quasi-stochasticity already.
# Our three constraints are: orthogonality, fixed diagonal, and non-negativity.␣
 ↪
@jax.jit
def obj1(V):
    O = jp.hstack([jp.ones((n,1))/jp.sqrt(n), V.reshape(n,r-1)])
    return jp.linalg.norm(O.T @ O - jp.eye(r)) +\
           jp.linalg.norm(jp.diag(O[:, 1:] @ O[:,1:].T) - jp.ones(n)*(r-1)/n) +\
           (jp.sum(O @ D @ O.T) - jp.sum(abs(O @ D @ O.T)))**2

result = sc.optimize.minimize(obj1, np.random.randn(n*(r-1)),\
                              jac=jax.jit(jax.jacrev(obj1)),\
                              #method="SLSQP",\
                              tol=1e-16, options={"disp": True, "maxiter": 10000})
O = jp.hstack([jp.ones((n,1))/jp.sqrt(n), result.x.reshape(n,r-1)]);
P = np.array(O @ D @ O.T); P
```

```
         Current function value: 0.000000
         Iterations: 115
         Function evaluations: 167
         Gradient evaluations: 164
```

```
/Users/heyredhat/opt/anaconda3/envs/spring2025/lib/python3.12/site-
packages/scipy/optimize/_minimize.py:733: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
  res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

[22]:
```
array([[0.417, 0.25 , 0.083, 0.25 ],
       [0.25 , 0.417, 0.25 , 0.083],
       [0.083, 0.25 , 0.417, 0.25 ],
       [0.25 , 0.083, 0.25 , 0.417]])
```

Let’s check out constraints are satisfied:

[23]:
```
np.all(P >= 0),\
np.allclose(u @ P, u),\
np.allclose(P @ u, u),\
np.allclose(P, P.T),\
np.allclose(np.diag(P), u/gamma),\
np.allclose(P @ Phi @ P, P),\
np.linalg.eigvals(P)
```

[23]:
```
(np.True_,
 True,
 True,
 True,
 True,
 True,
 array([ 1.    ,  0.333, -0.    ,  0.333]))
```

1.3 Generating valid probabilities

Our fundamental assumption which defines our state-space is that

$$P(E|\rho)\text{ valid} \iff \forall x \in \text{col}(P): \sum_i x_i^2 P(E_i|\rho) \geq \sum_{ijk} A_{ijk} x_i x_j P(E_k|\rho).$$

This becomes

$$\forall x \in \text{col}(P): \sum_{ij} x_i B[\rho]_{ij} x_j \geq 0,$$

if we let

$$B[\rho]_{ij} = \sum_k \Big(\delta_{ij}\delta_{ik} - A_{ijk}\Big) P(E_k|\rho),$$

or better yet, simply

$$C[\rho] \geq 0,$$

if we let $C[\rho] = P\Phi B[\rho] P\Phi$. In other words, $P(E|\rho)$ is valid iff $C[\rho]$ is positive-semidefinite.

It would be good to consider different choices of A_{ijk}, but for now let's stick to the choice that makes our theory as quantum-like as possible:

$$A_{ijk} = \eta\Big(\delta_{ij} - \delta_{ik} - \delta_{jk}\Big).$$

For simplicity, we'll take $\eta = -\frac{\beta}{\alpha+1}$: this can be derived by assuming an algebraic symmetry. We'll go with it at the moment to avoid another free parameter floating around.

With this estalished, we can then accumulate a list of valid probability-assignments by randomly generating probability vectors $P(E|\rho)$ and simply checking whether $C[\rho] \geq 0$.

[24]:
```
eta = -beta/(alpha+1)

delta = lambda i, j: 1 if i == j else 0
V = np.array([[[delta(i,j)*delta(i,k) for k in range(n)] for j in range(n)] for␣
 ↪i in range(n)])
```

```
A = np.array([[[eta*(delta(i,j) - delta(i,k) - delta(j,k)) for k in range(n)]␣
↪for j in range(n)] for i in range(n)])
B = lambda x: np.einsum("ijk, k", V-A, x)
C = lambda x: P @ Phi @ B(x) @ P @ Phi

def valid_probabilities(max_iter=1000):
    for i in range(max_iter):
        p = np.random.dirichlet(u)
        if np.all(np.linalg.eigvals(C(p)) >= 0):
            return p
    return u/n

p = valid_probabilities(); p
```

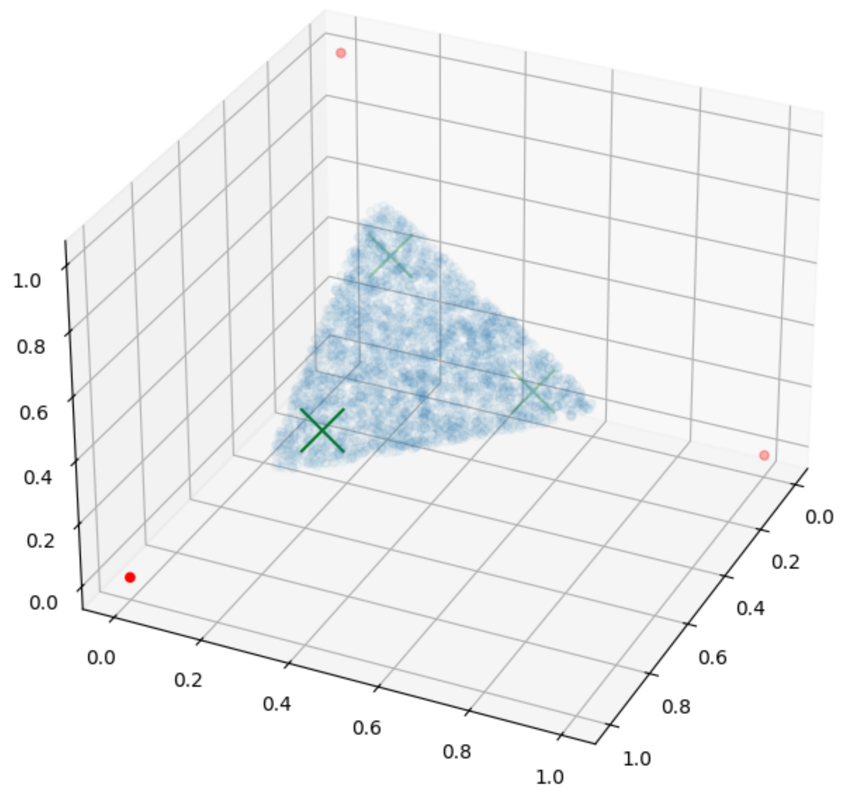
```
[24]: array([0.29 , 0.302, 0.269, 0.139])
```

1.3.1 Visualize 3D probability vectors

This works for $n = 3$. We generate some large number m of valid probablity vectors, and scatter-plot them in blue, along with the vertices of the probability simplex in red, and the probability vectors defining the reference (columns of P) in green. Try adjusting the opacity (alpha) to your taste.

```
[21]: %matplotlib widget

m = 3000
valid_ps = np.array([valid_probabilities() for i in range(m)]).T
simplex = np.eye(3)

fig = plt.figure(figsize=(8,8))
ax = fig.add_subplot(projection="3d")
ax.azim = 25

ax.scatter(*valid_ps, alpha=0.04)
ax.scatter(*simplex, c="r")
ax.scatter(*P, c="g", marker="x", s=500)
```

```
[21]: <mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x11afa69f0>
```



1.3.2 Visualize 4D probability vectors

This works when $n = 4$. In order to visualize this, we re-center the probability simplex around 0, and then embed into three dimensions. To implement this, we construct analysis and synthesis operators F, F^T. The idea is: 1. Re-center a probability vector around 0: $p_0 = p - \frac{1}{n}$. 2. Embed into 3D: $p' = Fp_0$. 3. Check that we can return: $F^T p' + \frac{1}{n} = p$.

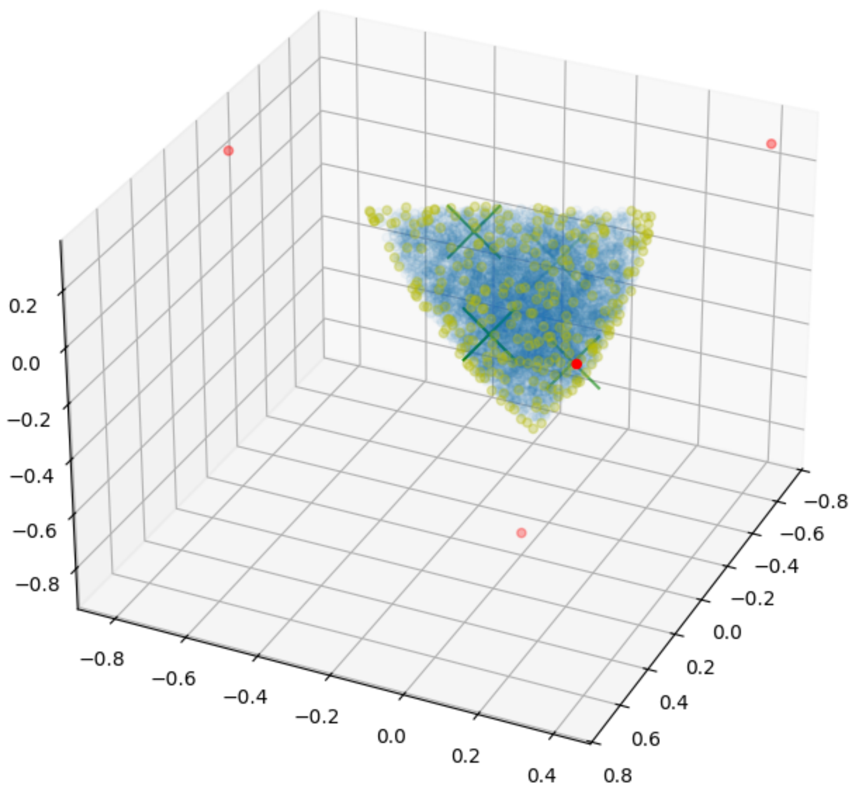
[25]:
```
simplex0 = np.eye(n) - u/n
L, D, R = np.linalg.svd(simplex0)
F = R[:-1,:]
np.allclose(simplex0, F.T @ F)
np.allclose(p, F.T @ (F @ (p - u/n)) + u/n)
```

```
[25]: True
```

Then as above, we scatter-plot the valid probability vectors, the simplex vectors, and the reference probability vectors. Additionally, using `scipy`, we calculate the convex hull of the valid vector, and plot them in yellow.

```
[26]: %matplotlib widget

m = 7000
valid_ps = np.array([valid_probabilities() for i in range(m)]).T
valid_ps_ = (F @ (valid_ps - np.ones(valid_ps.shape)/n))

hull = ConvexHull(valid_ps_.T)
hull_ps = valid_ps_.T[hull.vertices].T

simplex_ = (F @ (np.eye(n) - J/n))
P_ = (F @ (P - J/n))

fig = plt.figure(figsize=(8,8))
ax = fig.add_subplot(projection="3d")
ax.azim = 25

ax.scatter(*valid_ps_, alpha=0.04)
ax.scatter(*hull_ps, alpha=0.3, c="y")
ax.scatter(*simplex_, c="r")
ax.scatter(*P_, c="g", marker="x", s=750)
```

```
[26]: <mpl_toolkits.mplot3d.art3d.Path3DCollection at 0x11b0cef30>
```



1.4 Check self-duality

Okay, visualizing things is nice, but we're limited by the dimension. We can also try to analyze the state-space. For example, does every valid state also correspond to a valid effect? In other words, do we have $\forall \rho, \tau : P(E|\tau)\Phi P(E|\rho) \geq 0$?

[27]:
```
G = valid_ps.T @ Phi @ valid_ps
np.all(G >= 0)
```

[27]:
```
np.False_
```

[28]:
```
bad_guys = G < 0
```

```
[29]: G[bad_guys]
```

```
[29]: array([-0.018, -0.018, -0.04 , …, -0.005, -0.001, -0.004],
            shape=(112168,))
```

```
[30]: np.mean([bad_guys])
```

```
[30]: np.float64(0.002289142857142857)
```

1.5 Quantum 3-designs

Finally, for comparison, we can generate an actual quantum 3-design using similiar techniques, by minimizing the 3rd-order frame-potential. See if you can figure out what this code is doing!

```
[32]: d = 2 # 3
      n = 6 # 27
      t = 3

      @jax.jit
      def frame_potential(V):
          R = V[:d*n].reshape(d, n) + 1j*V[d*n:].reshape(d, n)
          R = R/jp.linalg.norm(R, axis=0)
          return (1/n**2)*jp.sum(abs(R.conj().T @ R)**(2*t))

      result = sc.optimize.minimize(frame_potential, np.random.randn(2*d*n),\
                                    jac=jax.jit(jax.jacrev(frame_potential)),\
                                    tol=1e-26,\
                                    options={"disp": True,\
                                             "maxiter": 10000})
      V = result.x
      R = V[:d*n].reshape(d, n) + 1j*V[d*n:].reshape(d, n)
      R = R/np.linalg.norm(R, axis=0)
      S = [np.outer(r, r.conj()) for r in R.T] # 3-design density matrices
      E = [(d/n)*e for e in S] # 3-design POVM elements
      P = np.array([[(e@s).trace() for s in S] for e in E]).real
      Phi = (d+1)*np.eye(n) - (d/n)*np.ones((n,n))
      P
```

```
         Current function value: 0.250000
         Iterations: 41
         Function evaluations: 74
         Gradient evaluations: 62

/Users/heyredhat/opt/anaconda3/envs/spring2025/lib/python3.12/site-
packages/scipy/optimize/_minimize.py:733: OptimizeWarning: Desired error not
necessarily achieved due to precision loss.
  res = _minimize_bfgs(fun, x0, args, jac, callback, **options)
```

```
[32]: array([[ 0.333,  0.167,  0.   ,  0.167,  0.167,  0.167],
             [ 0.167,  0.333,  0.167, -0.   ,  0.167,  0.167],
             [-0.   ,  0.167,  0.333,  0.167,  0.167,  0.167],
             [ 0.167, -0.   ,  0.167,  0.333,  0.167,  0.167],
             [ 0.167,  0.167,  0.167,  0.167,  0.333,  0.   ],
             [ 0.167,  0.167,  0.167,  0.167,  0.   ,  0.333]])
```