Accompaning notes for the neural network project for TBG in commensurate angles

1 Computing R^2 gradient

So we want to compute the gradient of R^2 as a function of the inputs. So we write:

$$R^2 = 1 - \frac{\sum_i (E(k_i) - E_p(k_i))^2}{\sum_i (E(k_i) - \mathbb{E}(E))^2} = 1 - \frac{\mathbb{E}((E - E_p)^2)}{\mathbb{E}((E - \mathbb{E}(E))^2)} \tag{1}$$

where we use the expected value notation

$$\mathbb{E}(f(k, E)) = \frac{1}{2N+1} \sum_{i=-N}^{N} f(i, E(k_i))$$

First, we want to compute the predicted value:

1.1 Computing the predicted value

We will assume that the points are given by

$$k_i = \mu + i\delta, \text{ for } i = -N, \dots, N$$

where δ is the sampling step size. We measure corresponding energies $E(k_i)$ and fit a linear model:

$$E_p(k) = \text{slope} \cdot k + \text{intercept}$$

We solve the linear system

$$\mathbf{A}\boldsymbol{\beta} = \mathbf{E}, \text{ where:}\mathbf{A} = \begin{bmatrix} k_{-N} & 1 \\ k_{-N+1} & 1 \\ \vdots & \vdots \\ k_N & 1 \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \text{slope} \\ \text{intercept} \end{bmatrix}, \quad \mathbf{E} = \begin{bmatrix} E_{-N} \\ E_{-N+1} \\ \vdots \\ E_N \end{bmatrix}$$

The normal equations give us: $\mathbf{A}^T\mathbf{A}\boldsymbol{\beta} = \mathbf{A}^T\mathbf{E}$.

So we compute $\mathbf{A}^T\mathbf{A}$. Since $k_i = \mu + i\delta$, we have:

$$\sum_{i=-N}^{N} k_i = \sum_{i=-N}^{N} (\mu + i\delta) = (2N+1)\mu + \delta \sum_{i=-N}^{N} i = (2N+1)\mu \tag{2}$$

$$\sum_{i=-N}^{N} k_i^2 = \sum_{i=-N}^{N} (\mu + i\delta)^2 = \sum_{i=-N}^{N} (\mu^2 + 2\mu i\delta + i^2\delta^2) \tag{3}$$

$$= (2N+1)\mu^2 + 2\mu\delta \sum_{i=-N}^{N} i + \delta^2 \sum_{i=-N}^{N} i^2 \tag{4}$$

$$= (2N+1)\mu^2 + \delta^2 \cdot \frac{N(N+1)(2N+1)}{3} \tag{5}$$

Let $\rho = \frac{N(N+1)}{3}$. Then:

$$\mathbf{A}^T\mathbf{A} = \begin{bmatrix} (2N+1)\mu^2 + \delta^2(2N+1)\rho & (2N+1)\mu \\ (2N+1)\mu & 2N+1 \end{bmatrix}$$

Now, we compute the determinant:

$$\begin{aligned} \det(\mathbf{A}^T\mathbf{A}) &= [(2N+1)\mu^2 + \delta^2(2N+1)\rho](2N+1) - [(2N+1)\mu]^2 \\ &= (2N+1)^2\mu^2 + \delta^2(2N+1)^2\rho - (2N+1)^2\mu^2 = \delta^2(2N+1)^2\rho \end{aligned}$$

and thus the inverse is:

$$(\mathbf{A}^T\mathbf{A})^{-1} = \frac{1}{\delta^2(2N+1)^2\rho} \begin{bmatrix} 2N+1 & -(2N+1)\mu \\ -(2N+1)\mu & (2N+1)\mu^2 + \delta^2(2N+1)\rho \end{bmatrix}$$

Simplifying:

$$(\mathbf{A}^T\mathbf{A})^{-1} = \frac{1}{\delta^2(2N+1)\rho} \begin{bmatrix} 1 & -\mu \\ -\mu & \mu^2 + \delta^2\rho \end{bmatrix}$$

Now, we can compute $(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T$:

$$\mathbf{A}^T = \begin{bmatrix} k_{-N} & k_{-N+1} & \cdots & k_N \\ 1 & 1 & \cdots & 1 \end{bmatrix}$$

The matrix multiplication gives:

$$(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T = \frac{1}{\delta^2(2N+1)\rho} \begin{bmatrix} 1 & -\mu \\ -\mu & \mu^2 + \delta^2\rho \end{bmatrix} \begin{bmatrix} k_{-N} & k_{-N+1} & \cdots & k_N \\ 1 & 1 & \cdots & 1 \end{bmatrix}$$

First row: For column i: $1 \cdot k_i + (-\mu) \cdot 1 = k_i - \mu = (\mu + i\delta) - \mu = i\delta$
Second row: For column i: $(-\mu) \cdot k_i + (\mu^2 + \delta^2\rho) \cdot 1 = -\mu(\mu + i\delta) + \mu^2 + \delta^2\rho = \delta^2\rho - \mu i\delta$
Therefore:

$$(\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T = \frac{1}{\delta(2N+1)\rho} \begin{bmatrix} -N & -N+1 & \cdots & N \\ \delta\rho + \mu N & \delta\rho + \mu(N-1) & \cdots & \delta\rho - \mu N \end{bmatrix}$$

This implies that the linear fit parameters will be:

$$\boldsymbol{\beta} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{E} = \frac{1}{\delta\rho(2N+1)} \begin{bmatrix} \sum_{i=-N}^{N} i \cdot E(k_i) \\ \delta\rho \sum_{i=-N}^{N} E(k_i) - \mu \sum_{i=-N}^{N} i \cdot E(k_i) \end{bmatrix}$$

Recall that

$$E_p(\mu + j\delta) = \text{slope} \cdot (\mu + j\delta) + \text{intercept}$$

Substituting our expressions:

$$E_p(\mu + j\delta) = \frac{1}{\delta\rho(2N+1)} \sum_{i=-N}^{N} i \cdot E(k_i) \cdot (\mu + j\delta) \tag{6}$$

$$+ \frac{1}{\delta\rho(2N+1)} \left[\delta\rho \sum_{i=-N}^{N} E(k_i) - \mu \sum_{i=-N}^{N} i \cdot E(k_i) \right] \tag{7}$$

$$= \frac{1}{\delta\rho(2N+1)} \left[\mu \sum_{i=-N}^{N} i \cdot E(k_i) + j\delta \sum_{i=-N}^{N} i \cdot E(k_i) + \delta\rho \sum_{i=-N}^{N} E(k_i) - \mu \sum_{i=-N}^{N} i \cdot E(k_i) \right] \tag{8}$$

$$= \frac{1}{\delta\rho(2N+1)} \left[j\delta \sum_{i=-N}^{N} i \cdot E(k_i) + \delta\rho \sum_{i=-N}^{N} E(k_i) \right] \tag{9}$$

$$= \frac{\delta}{\delta\rho(2N+1)} \left[j \sum_{i=-N}^{N} i \cdot E(k_i) + \rho \sum_{i=-N}^{N} E(k_i) \right] \tag{10}$$

Finally, we get that

$$E_p(\mu + j\delta) = \frac{j}{\rho(2N+1)} \sum_{i=-N}^{N} i \cdot E(k_i) + \frac{1}{2N+1} \sum_{i=-N}^{N} E(k_i)$$

Using the notation above, we have

$$E_p(k_j) = \frac{j}{\rho}\mathbb{E}(kE) + \mathbb{E}(E)$$
$$E_p = \frac{k}{\rho}\mathbb{E}(kE) + \mathbb{E}(E)$$

1.2 Simplified computation

We can now get a simplified version of R^2:

$$R^2 = 1 - \frac{\mathbb{E}[(E - \frac{k}{\rho}\mathbb{E}[kE] - \mathbb{E}[E]]^2)}{\mathbb{E}[(E - \mathbb{E}[E])^2]}$$
$$= 1 - \frac{\mathbb{E}[(E - \mathbb{E}[E])^2 - \frac{2k}{\rho}\mathbb{E}[kE](E - \mathbb{E}[E]) + \frac{k^2}{\rho^2}(\mathbb{E}[kE])^2]}{\mathbb{E}[(E - \mathbb{E}[E])^2]}$$
$$= 1 - \frac{\mathbb{E}[(E - \mathbb{E}[E])^2] - \frac{2}{\rho}\mathbb{E}[kE](\mathbb{E}[kE] - \mathbb{E}[k]\mathbb{E}[E]) + \frac{1}{\rho^2}(\mathbb{E}[kE])^2\mathbb{E}[k^2]}{\mathbb{E}[(E - \mathbb{E}[E])^2]}$$

Using that $\mathbb{E}[k] = 0, \mathbb{E}[k^2] = \rho$ we get that

$$R^2 = 1 - 1 + \frac{\frac{2}{\rho}\mathbb{E}[kE](\mathbb{E}[kE]) - \frac{1}{\rho}(\mathbb{E}[kE])^2}{\mathbb{E}[(E - \mathbb{E}[E])^2]} = \frac{1}{\rho}\frac{(\mathbb{E}[kE])^2}{\mathbb{E}[(E - \mathbb{E}[E])^2]}$$

So we conclude that

$$R^2 = \frac{1}{\rho}\frac{(\mathbb{E}[kE])^2}{\mathbb{E}[(E - \mathbb{E}[E])^2]} \tag{11}$$

And so we get that, using the fact that the derivative commutes with the expectation value

$$\nabla R^2 = \frac{1}{\rho}[\frac{2\mathbb{E}[kE]\mathbb{E}[k\nabla E]}{\mathbb{E}[(E-\mathbb{E}[E])^2]} - \frac{(\mathbb{E}[kE])^2}{\mathbb{E}[(E-\mathbb{E}[E])^2]}\frac{\mathbb{E}[2(E-\mathbb{E}[E])(\nabla E-\mathbb{E}[\nabla E])]}{\mathbb{E}[(E-\mathbb{E}[E])^2]}]$$

Focusing on the denominator of the second term, we have that

$$\begin{aligned}\mathbb{E}[(E-\mathbb{E}[E])(\nabla E-\mathbb{E}[\nabla E])] &= \mathbb{E}[E\nabla E] - \mathbb{E}[E]\mathbb{E}[\nabla E] - \mathbb{E}[E]\mathbb{E}[\nabla E] + \mathbb{E}[E]\mathbb{E}[\nabla E] \\ &= \mathbb{E}[E\nabla E] - \mathbb{E}[E]\mathbb{E}[\nabla E]\end{aligned}$$

So we conclude :

$$\begin{aligned}\nabla R^2 &= \frac{2}{\rho}[\frac{\mathbb{E}[kE]\mathbb{E}[k\nabla E]}{\mathbb{E}[(E-\mathbb{E}[E])^2]} - \rho R^2\frac{\mathbb{E}[E\nabla E]-\mathbb{E}[E]\mathbb{E}[\nabla E]}{\mathbb{E}[(E-\mathbb{E}[E])^2]}] \\ &= \frac{2}{\mathbb{E}[(E-\mathbb{E}[E])^2}[\frac{1}{\rho}\mathbb{E}[kE]\mathbb{E}[k\nabla E] - R^2(\mathbb{E}[E\nabla E]-\mathbb{E}[E]\mathbb{E}[\nabla E])]\end{aligned}$$

2 Computing the derivative of the isotropic measurement

The isotropy loss is defined as:

$$\text{iso\_loss} = \frac{\text{std(velocities)}}{\text{mean(velocities)}} = \frac{\sigma_v}{\mu_v}$$

where the velocities are the absolute values of the slopes from linear fits in different directions:

$$v_j = |\text{slope}_j| \quad \text{for direction } j = 1, 2, \ldots, N_{\text{dir}}$$

We recall the definitions:

$$\mu_v = \frac{1}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}} v_j \tag{12}$$

$$\sigma_v^2 = \frac{1}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}} (v_j - \mu_v)^2 \tag{13}$$

$$\sigma_v = \sqrt{\sigma_v^2} \tag{14}$$

So we can write

$$\nabla\left(\frac{\sigma_v}{\mu_v}\right) = \frac{\mu_v\nabla\sigma_v - \sigma_v\nabla\mu_v}{\mu_v^2}$$

let's first compute the derivative of μ_v:

$$\nabla\mu_v = \frac{1}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}}\nabla v_j = \frac{1}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}}\nabla|\text{slope}_j|$$

Next, we compute for σ_v:

$$\nabla\sigma_v = \frac{1}{2\sigma_v}\nabla(\sigma_v^2)$$

So we write:

$$\begin{aligned}\nabla(\sigma_v^2) &= \frac{1}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}}\nabla(v_j-\mu_v)^2 = \frac{1}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}}2(v_j-\mu_v)\left(\nabla v_j-\nabla\mu_v\right)\\ &= \frac{2}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}}(v_j-\mu_v)\nabla v_j - \frac{2}{N_{\text{dir}}}\nabla\mu_v\sum_{j=1}^{N_{\text{dir}}}(v_j-\mu_v)\end{aligned}$$

From our earlier derivation, the slope in direction j is:

$$\text{slope}_j = \frac{1}{\rho(2N+1)}\sum_{i=-N}^{N} i\cdot E_j(k_i)$$

and we have that $v_j = |\text{slope}_j|$, so we get that

$$\nabla v_j = \frac{\text{sgn}(\text{slope}_j)}{\rho(2N+1)}\sum_{i=-N}^{N} i\cdot\nabla E_j(k_i)$$

Putting it all together:

$$\begin{aligned}\nabla\text{iso}_{\text{loss}} &= \frac{1}{\mu_v^2}\left[\frac{\mu_v}{2\sigma_v}\frac{2}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}}(v_j-\mu_v)\nabla v_j - \sigma_v\frac{1}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}}\nabla v_j\right]\\ \nabla v_j &= \frac{\text{sgn}(\text{slope}_j)}{\rho(2N+1)}\sum_{i=-N}^{N} i\cdot\nabla E_j(k_i)\end{aligned}$$

We can simplify it:

$$\begin{aligned}\nabla\text{iso}_{\text{loss}} &= \frac{1}{N_{\text{dir}}\sigma_v}\left[\frac{1}{\mu_v}\sum_{j=1}^{N_{\text{dir}}}v_j\nabla v_j - [(\frac{\sigma_v}{\mu_v})^2+1]\sum_{j=1}^{N_{\text{dir}}}\nabla v_j\right]\\ &= \frac{1}{\sigma_v}\left[\frac{1}{\mu_v}\frac{1}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}}v_j\nabla v_j - [(\text{iso}_{\text{loss}})^2+1]\frac{1}{N_{\text{dir}}}\sum_{j=1}^{N_{\text{dir}}}\nabla v_j\right]\end{aligned}$$

3 On the symmetry of the problem

We will use the symmetry of the system to enhance our training data. First, we note that since the twist angle (which determines most of the physics) depends only on the ratio $\frac{\sqrt{3}b}{a}$, we can multiply a and b by the same factor and get the same result. So in the code, after each Dirac point found in say a, b, we will add data points with the same Dirac point, at $f\cdot a, f\cdot b$, for $f\in\{1,2,\ldots,9\}$

Second, we note that our system has symmetry of rotation by $\frac{\pi}{3}$, so we get that $H^{a,b}$ is our Hamiltonian as a function of a, b, then we have that

$$\begin{aligned}&\frac{\sqrt{3}b}{a} = \tan(\theta)\\ &\tan(\theta+\frac{\pi}{3}) = \sqrt{3}\frac{a+b}{a-3b}\end{aligned}$$

but since we restrict $a+b<a-3b \implies b<0$ Then it will be out of our scope.

We have another symmetry, which comes from the fact that our structure will be the same by flipping (other than swapping the labels of up and down). This will imply that we would care about

$$\frac{\sqrt{3}b}{a} = \tan(\theta)$$
$$\tan(\frac{\pi}{3}-\theta) = \sqrt{3}\frac{a-b}{a+3b}$$

So we get that

$$H^{a,b} \equiv H^{\tilde{a},\tilde{b}} = H^{a+3b,a-b}$$

First, we note that if $q \mid \tilde{a},\tilde{b}$, then we have that

$$q \mid a+3b, a-b \implies q \mid 4b$$

Then if $q \mid b$ and we have $q \mid a-b$ we get that $q \mid b,a \implies q=1$ as a,b are co-prime. So we conclude that $q \mid 4$. So we want to check if $2 \mid \tilde{a},\tilde{b}$. For that, we write

$$\alpha = 2^{\epsilon}(4\pi)^{\rho}, \epsilon = \begin{cases} 1, 2 \nmid ab \\ 0, \text{else} \end{cases}, \rho = \begin{cases} 1, 3 \mid a \\ 0, \text{else} \end{cases}$$

So we need to check two cases:

- If $\epsilon=0$, then $2 \nmid a-b, a+3b$ as only one of a,b is even, and so $\tilde{\epsilon}=1$.
- If $\epsilon=1$, then $2 \mid a-b, a+3b \implies 2 \mid \tilde{a},\tilde{b}$. In that case we need to consider $a'=\frac{a+3b}{2}, b'=\frac{a-b}{2}$. write

  $$a=4k+r, b=4\ell+r' \implies a'=2k+6\ell+\frac{r+3r'}{2}, b'=2k-2\ell+\frac{r-r'}{2}$$

  since $2 \nmid a,b$ we get that $r,r' \in \{\pm 1\}$. We note that if $r=r'$ we will get that we can take

  $$a''=\frac{a'}{2}=k+3\ell+r, b''=\frac{b'}{2}=k-\ell$$

  we note that one of a'',b'' has to be even, and so $\epsilon''=0$ (we note that if $3 \mid a''$ then $3 \mid a$). If $r \neq r'$, we ge that a',b' are both odd and so $\epsilon'=1$.

To conclude we get that if we define

$$\epsilon' = \begin{cases} 1, ab \equiv 1 \mod 4 \\ 0, \text{else} \end{cases}$$
$$\bar{a} = (a+3b)2^{-\epsilon-\epsilon'}$$
$$\bar{b} = (a-b)2^{-\epsilon-\epsilon'}$$

Then $\bar{a},\bar{b}$ are a co-prime representation of the equivalent angle.

We note that

$$3 \mid a \iff 3 \mid a-3b \iff 3 \mid \tilde{a} \iff 3 \mid \bar{a}$$

so we may conclude that $\bar{\rho} = \rho$.

Next, we note that

$$\bar{\epsilon} = 0 \iff \epsilon = 1, \epsilon' = 1 \implies \bar{\epsilon} = 1 - \epsilon\epsilon'$$

and so

$$\begin{aligned}\bar{N} &= \frac{1}{2^{\bar{\epsilon}}(4\pi)^{\bar{\rho}}}\sqrt{\bar{a}^2 + 3\bar{b}^2} = \frac{1}{2^{1-\epsilon\epsilon'}(4\pi)^{\rho}}\sqrt{(a+3b)^2 2^{-2\epsilon-2\epsilon'} + 3(a-b)^2 2^{-2\epsilon-2\epsilon'}} \\ &= \frac{2^{-\epsilon-\epsilon'}}{2^{1-\epsilon\epsilon'}(4\pi)^{\rho}}\sqrt{4a^2 + 12b^2} = \frac{2^{\epsilon'(\epsilon-\epsilon')}}{2^{\epsilon}(4\pi)^{\rho}}\sqrt{a^2 + 3b^2} = 2^{\epsilon'(\epsilon-\epsilon')}N\end{aligned}$$

Now we note that if $\epsilon = 0$ then $\epsilon' = 0$, so $(\epsilon - \epsilon') \neq 0$ only if $\epsilon = 1, \epsilon' = 0$, but then $\epsilon'(\epsilon - \epsilon') = 0$, so we conclude that $\bar{N} = N$ always. So we conclude that

$$H^{a,b} \equiv H^{(a+3b)2^{-\epsilon-\epsilon'},(a-b)2^{-\epsilon-\epsilon'}}$$