Dash for data visualization

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Who am I

- Twitter　https://twitter.com/iwatobipen
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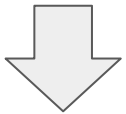
- 某製薬企業ケモインフォチームの中の人

Today’s topic

- Dashで簡単な可視化アプリを作ってみる

from Dash Introduction

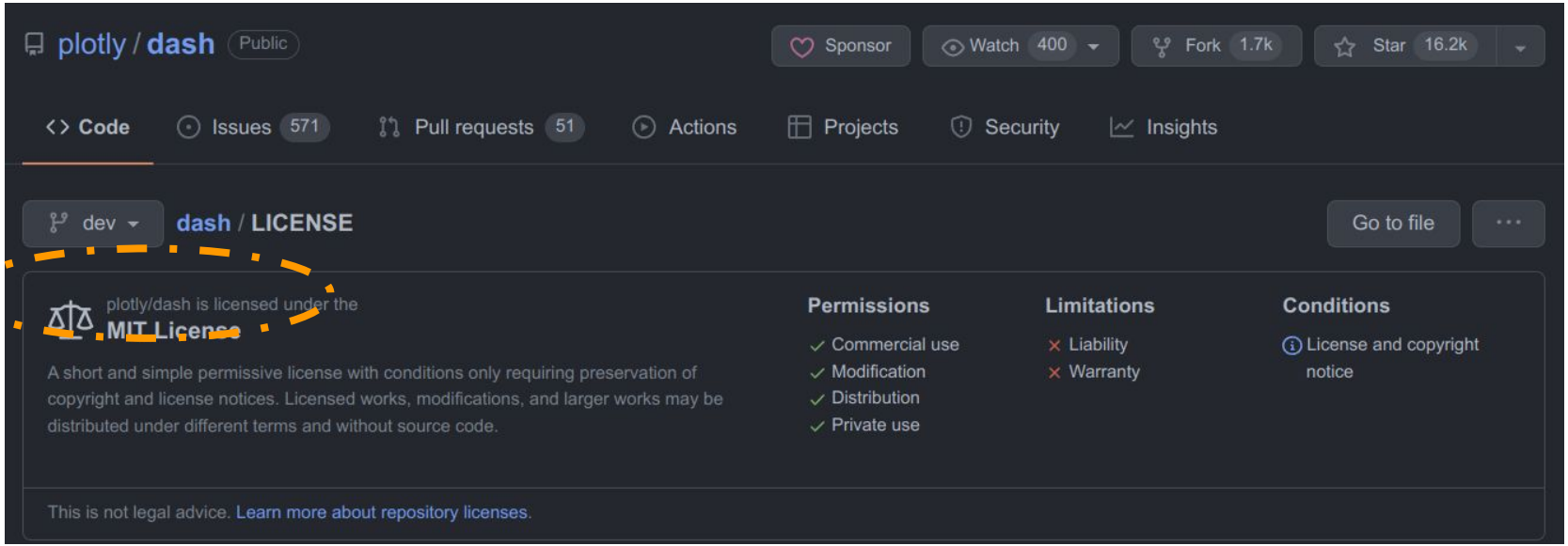
- Dash is the original low-code framework for rapidly building data apps in Python, R, Julia, and F# (experimental).
- Written on top of **Plotly.js** and **React.js,** Dash is ideal for **building and deploying data apps with customized user interfaces**. It's particularly suited for anyone who works with data.
- Dash is simple enough that you can bind a user interface to your code in less than 10 minutes.



- Dashはイケてるデータ可視化パッケージ（意訳）

https://dash.plotly.com/introduction

License MIT
(Enterpriseもある)



https://github.com/plotly/dash/blob/dev/LICENSE

Hello Dash!

```
#hello_world.py
from dash import Dash, html, dcc
app = Dash(__name__)

app.layout = html.Div(
    children=[html.H1("Hello Dash!")]
)
if __name__=="__main__":
    app.run_server(debug=True)
```

Flaskと同じお作法

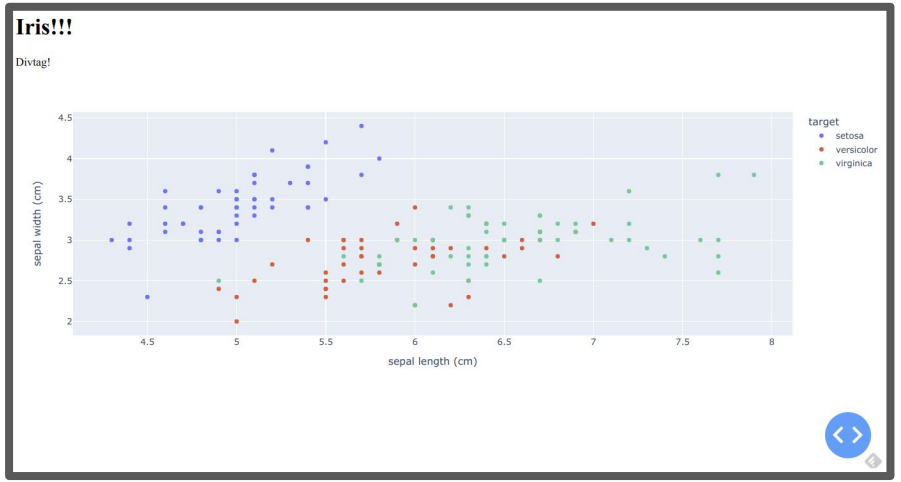
パーツをどんどん組み込む

http://localhost:8050/

Plot iris !!

```
#hello_plot.py
## snip
fig = px.scatter(df, x=data.feature_names[0],
     y=data.feature_names[1], color='target')
app = Dash(__name__)
app.layout = html.Div(children=[
    html.H1(children='Iris!!!'),
    html.Div(children="Divtag!"),
    dcc.Graph(  id="iris!", figure=fig)])
## snip
```

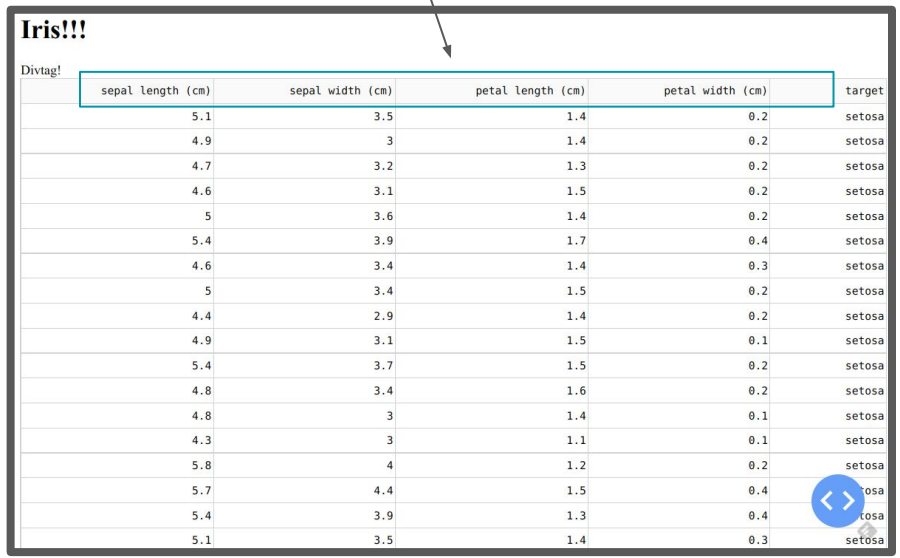
Plotlyできれいなプロット♪



Iris dataset has 4 features…

```
#hello_table.py

## snip

from dash import dash_table

app = Dash(__name__)

app.layout = html.Div(children=[

    html.H1(children='Iris!!!'),

    html.Div(children="Divtag!"),

    dash_table.DataTable(df.to_dict('records'),
[{"name": i, "id": i} for i in df.columns])

    ])
```

この4つを任意に選んでプロットしたいよね



Iris!!!

Divtag!

	sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	target
	5.1	3.5	1.4	0.2	setosa
	4.9	3	1.4	0.2	setosa
	4.7	3.2	1.3	0.2	setosa
	4.6	3.1	1.5	0.2	setosa
	5	3.6	1.4	0.2	setosa
	5.4	3.9	1.7	0.4	setosa
	4.6	3.4	1.4	0.3	setosa
	5	3.4	1.5	0.2	setosa
	4.4	2.9	1.4	0.2	setosa
	4.9	3.1	1.5	0.1	setosa
	5.4	3.7	1.5	0.2	setosa
	4.8	3.4	1.6	0.2	setosa
	4.8	3	1.4	0.1	setosa
	4.3	3	1.1	0.1	setosa
	5.8	4	1.2	0.2	setosa
	5.7	4.4	1.5	0.4	setosa
	5.4	3.9	1.3	0.4	setosa
	5.1	3.5	1.4	0.3	setosa

Let's use callback

```
from dash import Dash, dcc, html, Input, Output
app = Dash(__name__)
app.layout = html.Div([
    html.H6("Callbacks in action!"),
    html.Div([
        "Input: ",
        dcc.Input(id='my-input', value='initial value', type='text')
    ]),
    html.Br(),
    html.Div(id='my-output'),
])

@app.callback(
   Output(component_id='my-output',
    component_property='children'),
    Input(component_id='my-input', component_property='value'))
def update_output_div(input_value):
    return f'Output: {input_value}'
if __name__ == '__main__':
    app.run_server(debug=True)
```

dcc以下に様々な入力用のクラスがある

入出力をCallBack側で制御。

https://dash.plotly.com/basic-callbacks

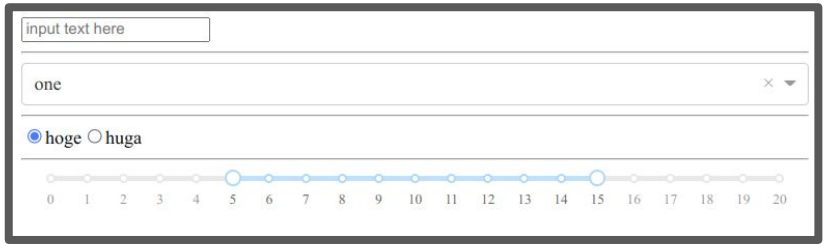
There are lots of parts in dcc ;)

dcc.Dropdown	ドロップダウンリストの実装に	散布図の軸選択
dcc.Input	テキスト入力に	
dcc.Slider	スライダーで数値指定	
dcc.Upload	ファイルアップロード	SDFをアップロードとか
dcc.RadioItems	ラジオボタン	項目選択に
dcc.RangeSlider	x〜yのようなレンジでの選択	分子物性の選択などに
などなど。。。		

https://dash.plotly.com/dash-core-components

dcc examples

```
# dcc_sample.py

from dash import Dash, dcc, html

app = Dash(__name__)

app.layout = html.Div(children=[
    dcc.Input(id='input', placeholder='input text here'),
    dcc.Dropdown(['one', 'two', 'three'], 'one', id='dropdown'),
    dcc.RadioItems(['hoge', 'huga'], 'hoge'),
    dcc.RangeSlider(0, 20, 1, value=[5,15],id='rangeslider')
])

if __name__=="__main__":
    app.run_server(debug=True)
```

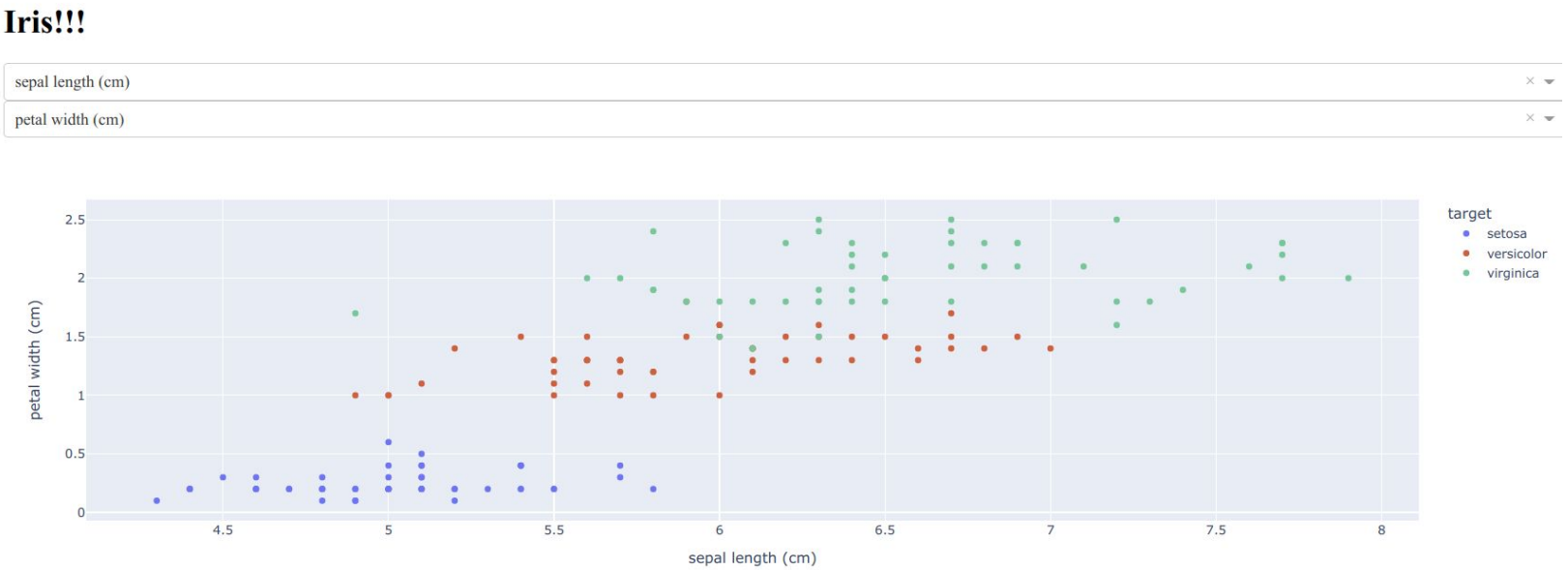


Interactive plot of Iris ;-)

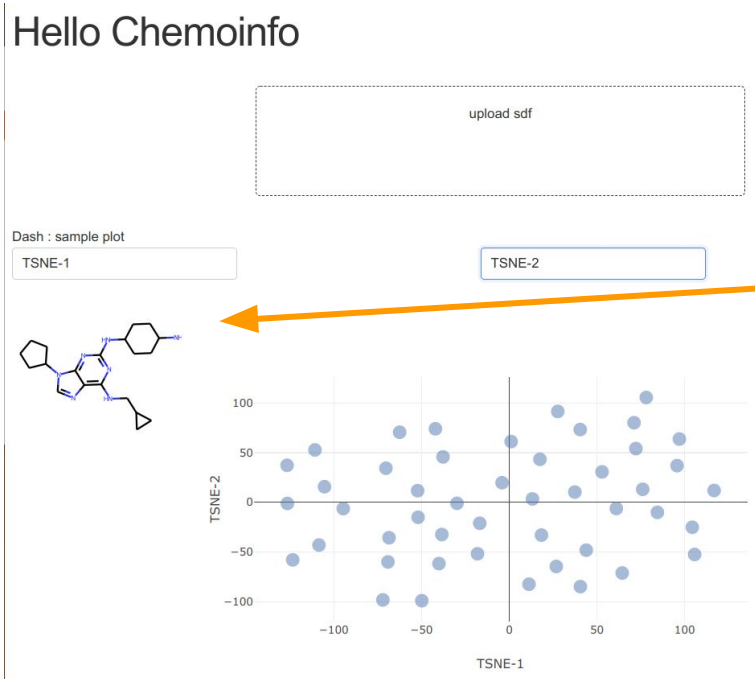
app.layoutをCallbackの方で制御する
＞id属性でデータを紐付け

```
# hello_plot_v2.py
app = Dash(__name__)
app.layout = html.Div(children=[html.H1(children='Iris!!!'),
    dcc.Dropdown(data.feature_names, id='x-axis'),
    dcc.Dropdown(data.feature_names, id='y-axis'),
    dcc.Graph(id="iris")])
@app.callback(Output('iris', 'figure'), Input('x-axis', 'value'), Input('y-axis', 'value'))
def updatefig(xval, yval):
    fig = px.scatter(df,  x=xval, y=yval, color='target')
    return fig
```

Interactive plot of Iris ;-)



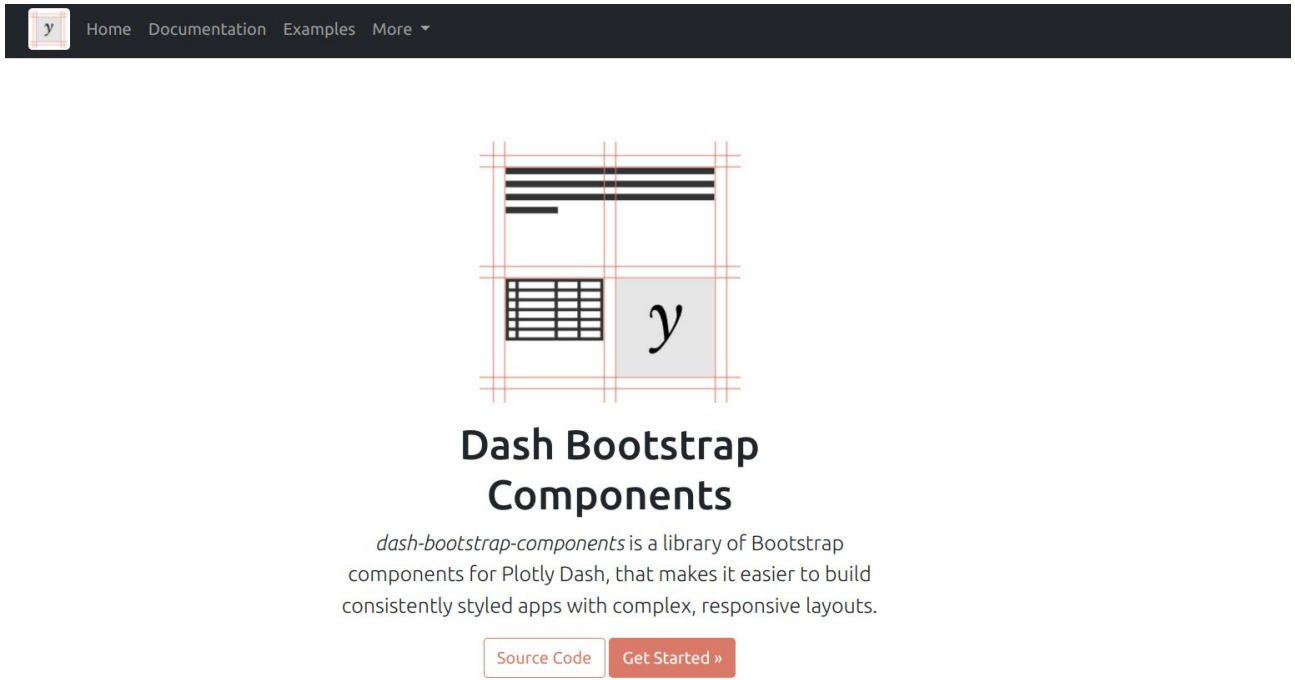
Chemoinfo appも作れるよ




```
app.layout = html.Div(children=[
    html.H1(children='Hello Chemoinfo'),
        dcc.Upload(
            id='sdf',
            children=html.Div(['upload sdf']),
            style=upload_style,
        ),

    html.Div(children='''
    Dash : sample plot
    '''),

    html.Div([dcc.Dropdown(id='x-column',
                           value='PC-1',
                           options=[{'label': key, 'value': key} for key in vals.keys()],
                           style={'width':'48%', 'display':'inline-block'}),
              dcc.Dropdown(id='y-column',
                           value='PC-2',
                           options=[{'label': key, 'value': key} for key in vals.keys()],
                           style={'width':'48%', 'display':'inline-block'}),
                           ]),
    html.Div([
        html.Div([html.Div(id="molimg")], className="two columns"),
        html.Div([dcc.Graph(id='mol_graph')], className="eight columns")
        ],
        className="row"
        ),
```

```
@app.callback(
    Output('molimg', 'children'),
    [Input('mol_graph', 'hoverData'),
    ]
)
def update_img(hoverData):
    try:
        svg = smi2svg(hoverData['points'][0]['text'])
    except:
        svg = 'Select molecule'
    return dhtml.DangerouslySetInnerHTML(svg)
```

もう少しレイアウトをという方にはこちら！

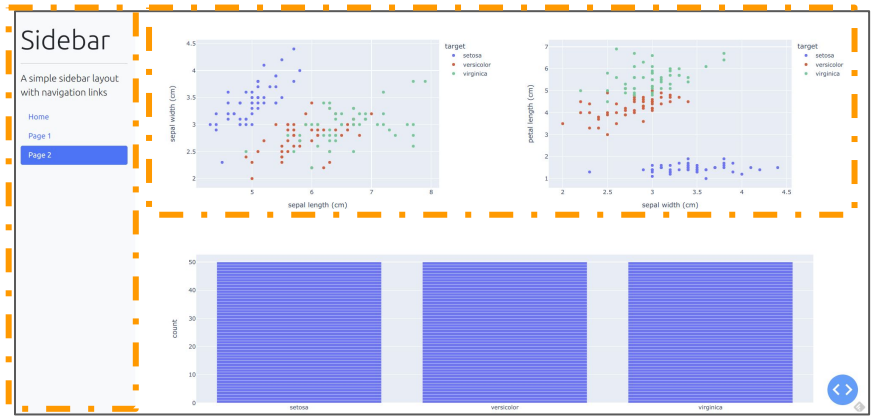


https://dash-bootstrap-components.opensource.faculty.ai/

#sidebar_with_graph.py

DBCを使ってレイアウトを簡単にコントロール

```
sidebar = html.Div(
    [
        html.H2("Sidebar", className="display-4"),
        html.Hr(),
        html.P(
            "A simple sidebar layout with navigation links", className="lead"
        ),
        dbc.Nav(
            [
                dbc.NavLink("Home", href="/", active="exact"),
                dbc.NavLink("Page 1", href="/page-1", active="exact"),
                dbc.NavLink("Page 2", href="/page-2", active="exact"),
            ],
            vertical=True,
            pills=True,
        ),
    ],
    style=SIDEBAR_STYLE,
)


content = html.Div(
    [
        dbc.Row(
            [
                dbc.Col([html.P('scatter plot1'),dcc.Graph(id='fig1',figure=fig1)], width=6),
                dbc.Col([html.P('scatter plot2'),dcc.Graph(id='fig2', figure=fig2)], width=6)
```



12のColumnで構成されるGridレイアウト

ところで、、、、

- 既存のFlask Appがもうあるんだけど、Dashをそこに組み込めたりしないの？
- サービスが全部独立してしまうのはちょっと、、、

という貴方に！！！

```
from dash import Dash
from werkzeug.middleware.dispatcher import DispatcherMiddleware
from werkzeug.serving import run_simple
import flask
from flask import Flask
from dash import html
server = Flask(__name__)

dash_app1 = Dash(__name__, server = server, url_base_pathname='/dashboard/' )
dash_app2 = Dash(__name__, server = server, url_base_pathname='/reports/')
dash_app1.layout = html.Div([html.H1('Hi there, I am app1 for dashboards')])
dash_app2.layout = html.Div([html.H1('Hi there, I am app2 for reports')])

@server.route('/dashboard/')
def render_dashboard():
    return flask.redirect('/dash1')

@server.route('/reports/')
def render_reports():
    return flask.redirect('/dash2')
app = DispatcherMiddleware(server, {
    '/dash1': dash_app1.server,
    '/dash2': dash_app2.server,})

run_simple('localhost', 8080, app, use_reloader=True, use_debugger=True)
```

その他参考情報
☆PatWalterさんのBlogは要チェック！

- https://practicalcheminformatics.blogspot.com/2019/11/interactive-plots-with-chemical.html
- https://iwatobipen.wordpress.com/2022/02/20/integration-of-molplotly-and-flask-for-developing-chemoinformatics-web-app-rdkit-molplotly-flask/
- https://github.com/wjm41/molplotly
-

まとめ

- Dashを使って良さげな可視化を提供しよう！
- リッチな可視化を提供する場合Call backやLayoutなどそこそこコード書く必要はあるが、フルスクラッチで開発するよりはコストが低い
- Plotlyのプロットきれいで動的なの良いですね
- 企業であれば便利なBIツールを使うかな
- 今日のコードと資料はMishima-sykリポジトリをチェケ！

https://github.com/Mishima-syk/18/tree/main/iwatobipen

おしまい