

Introduction to Optimal Decision Making

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Contents

1	Introduction	1
2	Motivation	3
2.1	Optimal Decision Making. Why and how?	3
2.2	Optimal decisions with different types of model	3
3	Cost-sensitive classification	5
3.1	Cost matrices: Binary example	5
3.2	Cost Matrix “reasonableness” condition	7
3.3	Optimal threshold for the binary case	8
3.4	Different costs binary example	10
3.5	Cost invariances	13
3.6	Multiclass setting	16
3.7	Ternary example {smaller}	17
3.8	Option to abstain	20

1 Introduction

This is an introductory course on the topic of **Optimal Decision Making** for multiclass classification. In Section 2, we give some motivation insights about the importance of estimating missclassification costs when making automatic decisions, then we define a common setting to calculate expected costs and how to make an optimal decision based on those expected costs in the binary (Section 3.1) and multiclass (Section 3.6) case. We provide interactive examples that demonstrate how the optimal decision change under different operational conditions. Finally in Section 3.8, we demonstrate examples in which abstaining on making a prediction and delegating the decision may be optimal solution.

2 Motivation

2.1 Optimal Decision Making. Why and how?

One of the most common objectives of multiclass classification is to train a machine learning model that is able to predict the most probable class given a new instance. However, in certain applications in which the missclassification costs are of main importance, the most probable class may not be the one that provides the highest expected utilities. The objective of optimal decision making is to predict the class that maximises the expected utilities, and minimises the expected missclassification costs. Some typical scenarios in which this is important are medical diagnosis, self-driving cars, extreme weather prediction and finances.

2.1.1 Key points

- The objective is to classify a new instance into one of the possible classes in an optimal manner.
- This may be important in critical applications: e.g. medical diagnosis [2, 16], self-driving cars [14, 11], extreme weather prediction, finances [12].



- It is necessary to know what are the consequences of making each prediction (costs or gains).
- One way to make optimal decisions is with cost-sensitive classification.
- Can we make optimal decisions with any type of classifier?

2.2 Optimal decisions with different types of model

- **Class estimation:** Outputs a class prediction.
- **Class estimation with option of abstaining:** Outputs a class prediction or abstains [5, 10]

2 Motivation

- **Rankings estimation:** Outputs a ranked list of possible classes [3].
- **Score surrogates:** Outputs a continuous score which is commonly a surrogate for classification (e.g. Support Vector Machines).
- **Probability estimation:** Outputs class posterior probability estimates (e.g. Logistic Regression, naive Bayes, Artificial Neural Networks), or provides class counts which can be interpreted as proportions (e.g. decision trees, random forests, k-nearest neighbour) [17].
- **Other types of outputs:** Some examples are possibility theory [7], credal sets [9], conformal predictions [15], multi-label [1].

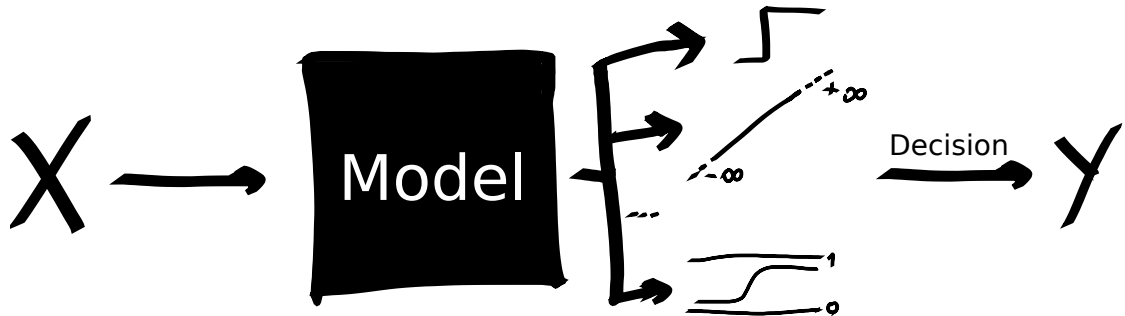


Figure 2.1: Classifier as a black box

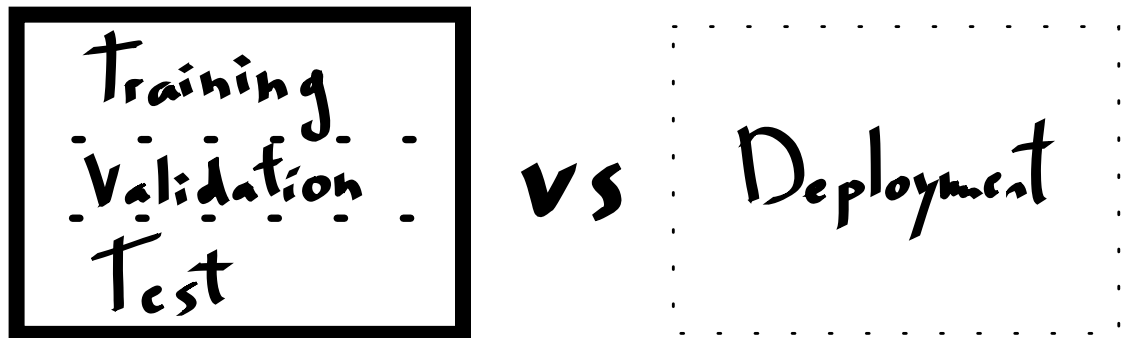


Figure 2.2: Training vs Deployment

3 Cost-sensitive classification

- Cost-sensitive classification [8] provides a framework to make optimal decisions (with certain assumptions).
- We require the true posterior probabilities of each outcome in order to make optimal decisions, but we can use estimates.
- Assumes the costs are not instance dependent (only depend on the predicted and true class).
- Class priors and costs can be changed during deployment (if known or estimated).

3.1 Cost matrices: Binary example

The following is a typical example of a cost matrix c for a binary problem.

	Predicted C_1	Predicted C_2
True C_1	0	1
True C_2	1	0

We will refer to $c_{i|j}$ the cost of predicting class C_i given that the true class is C_j .

Given the posterior probabilities $P(C_j|\mathbf{x})$ where $j \in \{1, K\}$ and the cost matrix c we can calculate the expected cost of predicting class C_i

$$\mathbb{E}_{j \sim P(\cdot|\mathbf{x})}(c_{i|j}) = \sum_{j=1}^K P(C_j|\mathbf{x})c_{i|j}. \quad (3.1)$$

For example, let's assume that the posterior probability vector for a given instance is $[0.4, 0.6]$, the expected costs will be

- Predicting **Class 1** will have an expected cost of $0.4 \times 0 + 0.6 \times 1 = 0.6$
- Predicting **Class 2** will have an expected cost of $0.4 \times 1 + 0.6 \times 0 = 0.4$.

3.1.1 Expected costs figure

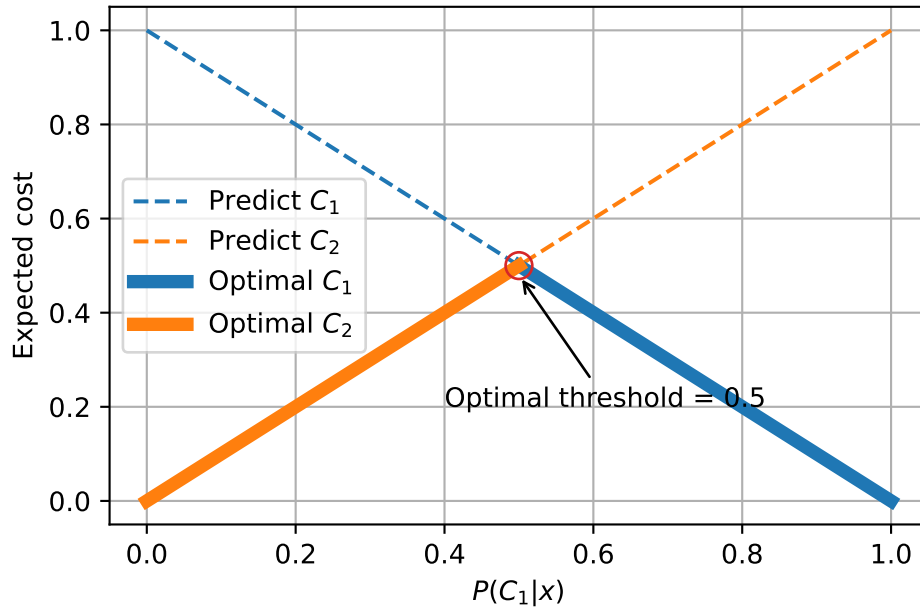
We can visualise the cost lines for each prediction with a line for each predicted class C_i and its missclassification costs and correct predictions [6]. For example, the following cost matrix

	Predicted C_1	Predicted C_2
True C_1	0	1
True C_2	1	0

will result in the following cost lines

```
import matplotlib.pyplot as plt

C = [[0, 1], [1, 0]]
threshold = (C[0][1] - C[1][1]) / (C[0][1] - C[1][1] + C[1][0] - C[0][0])
cost_t = threshold * C[0][0] + (1 - threshold) * C[0][1]
plt.grid(True)
plt.plot([0, 1], [C[0][1], C[0][0]], '--', label="Predict $C_1$")
plt.plot([0, 1], [C[1][1], C[1][0]], '--', label="Predict $C_2$")
plt.plot([threshold, 1], [cost_t, C[0][0]], lw=5, color='tab:blue', label="Optimal")
plt.plot([0, threshold], [C[1][1], cost_t], lw=5, color='tab:orange', label="Optimal")
plt.xlabel('$P(C_1|x)$')
plt.ylabel('Expected cost')
plt.legend()
plt.annotate("Optimal threshold = 0.5", (0.5, 0.48), xytext=(0.4, 0.2),
            arrowprops=dict(arrowstyle='->', facecolor='black'))
plt.scatter(0.5, 0.5, s=100, facecolors='none', edgecolors='tab:red', zorder=10)
plt.show()
```



where we have highlighted the minimum cost among the possible predictions. In this particular case the optimal prediction changes when the probability of the true class is higher or lower than 0.5, with the same expected cost for both classes at 0.5.

3.2 Cost Matrix “reasonableness” condition

In general, it is reasonable to expect cost matrices where:

1. For a given class j the correct prediction has always a lower cost than an incorrect prediction $c_{j|j} < c_{i|j}$ with $i \neq j$.
2. **Class domination:** One class does not consistently have lower costs than other classes $c_{i|j} \leq c_{k|j}$ for all j .

We will make these reasonable assumptions in this introductory module.

3.2.1 Class Domination

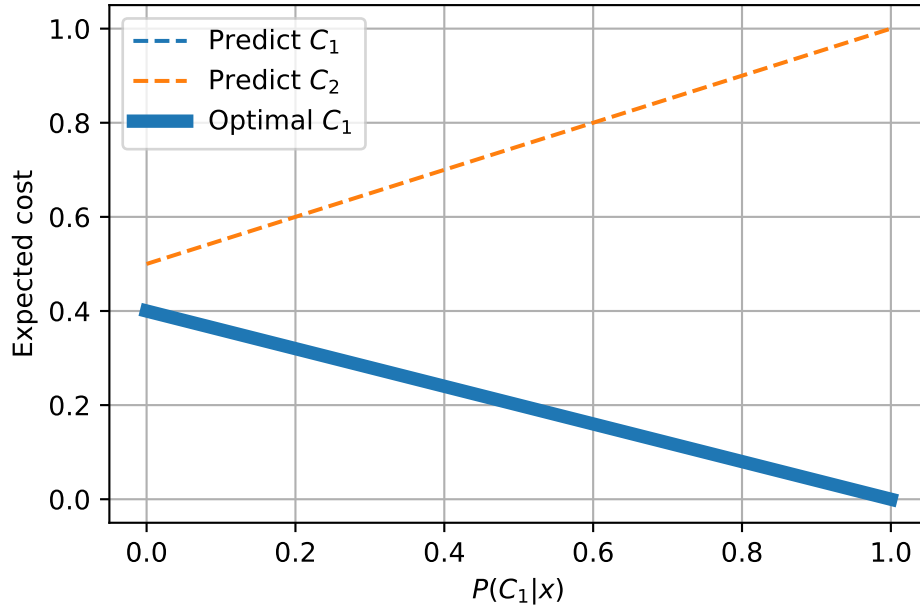
The following is an example of class domination in which predicting class C_1 will always have a lower expected cost.

3 Cost-sensitive classification

	Predicted C_1	Predicted C_2
True C_1	0	1
True C_2	0.4	0.5

```
import matplotlib.pyplot as plt

plt.grid(True)
plt.plot([0, 1], [0.4, 0], '--', color='tab:blue', label="Predict  $C_1$ ")
plt.plot([0, 1], [0.5, 1], '--', color='tab:orange', label="Predict  $C_2$ ")
plt.plot([0, 1], [0.4, 0], lw=5, color='tab:blue', label="Optimal  $C_1$ ")
plt.xlabel('$P(C_1|x)$')
plt.ylabel('Expected cost')
plt.legend()
plt.show()
```



3.3 Optimal threshold for the binary case

If we know the true posterior probabilities, the optimal decision is to choose the class that minimizes the expected cost which can be obtained by marginalising the predicted class over all possible true classes [13].

3.3 Optimal threshold for the binary case

$$\hat{y}(\mathbf{x}) = \arg \min_{i=\{1,\dots,K\}} \mathbb{E}_{j \sim P(\cdot|\mathbf{x})}(c_{i|j}) = \arg \min_{i=\{1,\dots,K\}} \sum_{j=1}^K P(C_j|\mathbf{x})c_{i|j}. \quad (3.2)$$

In the binary case we want to predict class C_1 if and only if predicting class C_1 has a lower expected cost than predicting class C_2

$$\sum_{j=1}^K P(C_j|\mathbf{x})c_{1|j} \leq \sum_{j=1}^K P(C_j|\mathbf{x})c_{2|j} \quad (3.3)$$

$$P(C_1|\mathbf{x})c_{1|1} + P(C_2|\mathbf{x})c_{1|2} \leq P(C_1|\mathbf{x})c_{2|1} + P(C_2|\mathbf{x})c_{2|2} \quad (3.4)$$

$$(3.5)$$

with the equality having the same expected cost independent on the predicted class.

$$pc_{1|1} + (1-p)c_{1|2} = pc_{2|1} + (1-p)c_{2|2} \quad (3.6)$$

where $p = P(C_1|\mathbf{x})$.

In the binary classification setting we can derive the optimal threshold t^* of selecting class one if $p \geq t^*$.

$$t^*c_{1|1} + (1-t^*)c_{1|2} = t^*c_{2|1} + (1-t^*)c_{2|2} \quad (3.7)$$

$$(1-t^*)c_{1|2} - (1-t^*)c_{2|2} = t^*c_{2|1} - t^*c_{1|1} \quad (3.8)$$

$$(1-t^*)(c_{1|2} - c_{2|2}) = t^*(c_{2|1} - c_{1|1}) \quad (3.9)$$

$$(c_{1|2} - c_{2|2}) - t^*(c_{1|2} - c_{2|2}) = t^*(c_{2|1} - c_{1|1}) \quad (3.10)$$

$$(c_{1|2} - c_{2|2}) = t^*(c_{2|1} - c_{1|1}) + t^*(c_{1|2} - c_{2|2}) \quad (3.11)$$

$$(c_{1|2} - c_{2|2}) = t^*(c_{2|1} - c_{1|1} + c_{1|2} - c_{2|2}) \quad (3.12)$$

$$\frac{c_{1|2} - c_{2|2}}{c_{2|1} - c_{1|1} + c_{1|2} - c_{2|2}} = t^* \quad (3.13)$$

For the previous cost matrix

3 Cost-sensitive classification

	Predicted C_1	Predicted C_2
True C_1	0	1
True C_2	1	0

the optimal threshold corresponds to

$$t^* = \frac{c_{1|2} - c_{2|2}}{c_{1|2} - c_{2|2} + c_{2|1} - c_{1|1}} = \frac{1 - 0}{1 + 1 - 0 - 0} = 0.5 \quad (3.14)$$

3.4 Different costs binary example

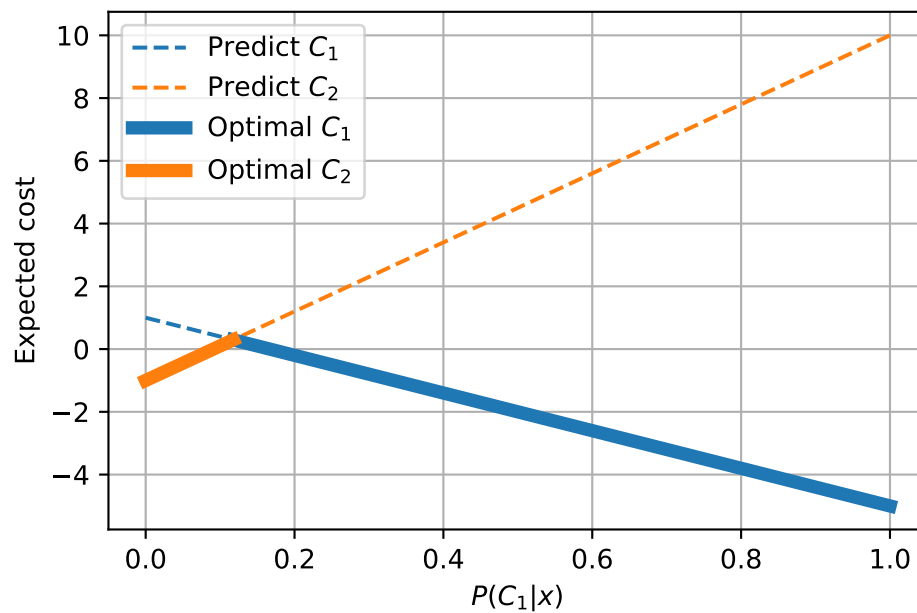
In general, the correct predictions have a cost of 0. However, this may be different in certain scenarios. The following is an example of a cost matrix with different **gains** on the main diagonal and missclassification costs.

	Predicted C_1	Predicted C_2
True C_1	-5	10
True C_2	1	-1

which would result in the following cost lines.

```
import matplotlib.pyplot as plt

C = [[-5, 1], # TP, FN
      [10, -1]] # FP, TN
threshold = (C[0][1] - C[1][1]) / (C[0][1] - C[1][1] + C[1][0] - C[0][0])
cost_t = threshold * C[0][0] + (1 - threshold) * C[0][1]
plt.grid(True)
plt.plot([0, 1], [C[0][1], C[0][0]], '--', label="Predict $C_1$")
plt.plot([0, 1], [C[1][1], C[1][0]], '--', label="Predict $C_2$")
plt.plot([threshold, 1], [cost_t, C[0][0]], lw=5, color='tab:blue', label="Optimal")
plt.plot([0, threshold], [C[1][1], cost_t], lw=5, color='tab:orange', label="Optimal")
plt.xlabel('$P(C_1|x)$')
plt.ylabel('Expected cost')
plt.legend()
plt.show()
```



In this case, for a posterior probability vector $[0.4, 0.6]$ we would expect

- Predicting **Class 1** will have an expected cost of $-5 \times 0.4 + 1 \times 0.6 = -1.4$
- Predicting **Class 2** will have an expected cost of $10 \times 0.4 - 1 \times 0.6 = 3.4$

3.4.1 Other binary examples

```
import matplotlib.pyplot as plt
from shiny import App, render, ui
import pandas as pd

TP = -5
FN = 10
FP = 1
TN = -1
fig = plt.figure()
ax = fig.add_subplot()
ax.grid(True)
ax.plot([0, 1], [FP, TP], '--', label="Predict $C_1$")
ax.plot([0, 1], [TN, FN], '--', label="Predict $C_2$")
```

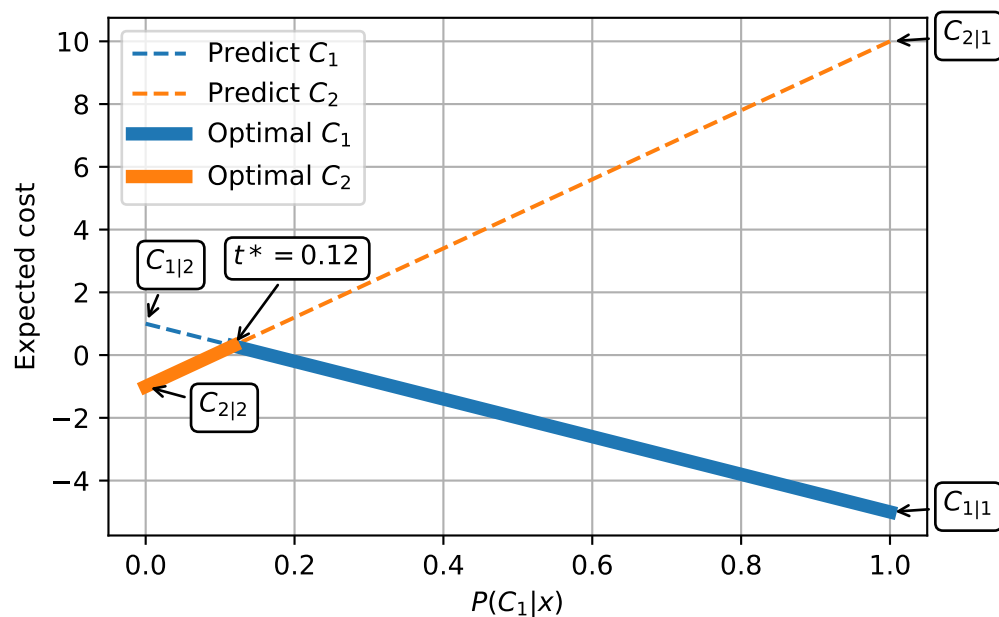
3 Cost-sensitive classification

```
threshold = (FP - TN)/(FP - TN + FN - TP)
cost_t = threshold*TP + (1-threshold)*FP
ax.plot([threshold, 1], [cost_t, TP], lw=5, color='tab:blue', label="Optimal $C_1$"
ax.plot([0, threshold], [TN, cost_t], lw=5, color='tab:orange', label="Optimal $C_2$")

C = [[TP, FP], [FN, TN]]
bbox = dict(boxstyle="round", fc="white")
ax.annotate(r'$C_{2|2}$', (0, C[1][1]), xytext=(2, -1),
            textcoords='offset fontsize',
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)
ax.annotate(r'$C_{1|1}$', (1, C[0][0]), xytext=(2, 0),
            textcoords='offset fontsize',
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)
ax.annotate(r'$C_{1|2}$', (0, C[0][1]), xytext=(0, 2),
            textcoords='offset fontsize',
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)
ax.annotate(r'$C_{2|1}$', (1, C[1][0]), xytext=(2, 0),
            textcoords='offset fontsize',
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)

ax.annotate(f'$t*=\{threshold:0.2\}$', (threshold, cost_t),
            xytext=(0, --3),
            textcoords='offset fontsize',
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)

ax.set_xlabel('$P(C_1|x)$')
ax.set_ylabel('Expected cost')
ax.legend()
```

3.5 Cost invariances

The optimal prediction does not change if the cost matrix is

- Multiplied by a positive constant value
- Shifted by a constant value

```

#| standalone: true
#| components: viewer
#| viewerHeight: 480

import numpy as np
import matplotlib.pyplot as plt
from shiny import App, render, ui
import pandas as pd

def fraction_to_float(fraction):
    if '/' in fraction:
        numerator, denominator = fraction.split('/')
        result = float(numerator)/float(denominator)
    else:
        result = float(fraction)

```

3 Cost-sensitive classification

```
    return result

# X|Y means predict X given that the true label is Y
# Because the indices in a matrix are first row and then column we need to
# invert the order of X and Y by transposing the matrix. Then [0,1] is predict 0
# when the true label is 1.
# TODO: check indices
C_original = np.array([[ -2,  3],      # 1|1, 2|1
                       [13, -7]]).T  # 1|2, 2|2

app_ui = ui.page_fluid(
    ui.layout_sidebar(
        ui.panel_sidebar(
            ui.input_slider("S", "Shift constant S", value=0, min=-10,
                           max=10),
            ui.input_radio_buttons("M", "Multiplicative constant M",
                                   choices=['1/20', '1/10', '1/5', '1',
                                           '5', '10', '20'],
                                   selected = '1', inline=True, width='100%'),
            ui.output_table('cost_matrix'),
        ),
        ui.panel_main(
            ui.output_plot("plot")
        )
    ),
)

def server(input, output, session):
    @output
    @render.plot(alt="A histogram")
    def plot():
        fig = plt.figure()
        ax = fig.add_subplot()
        ax.grid(True)

        global C_original
        C = C_original + input.S()
        C = C*fraction_to_float(input.M())

        threshold = (C[0][1] - C[1][1])/(C[0][1] - C[1][1] + C[1][0] - C[0][0])
        cost_t = threshold*C[0][0] + (1-threshold)*C[0][1]

        ax.plot([0, 1], [C[0][1], C[0][0]], '--', label="Predict $C_1$")
```

```

ax.plot([0, 1], [C[1][1], C[1][0]], '--', label="Predict $C_2$")
ax.plot([threshold, 1], [cost_t, C[0][0]], lw=5, color='tab:blue', label="Optimal $C_1$")
ax.plot([0, threshold], [C[1][1], cost_t], lw=5, color='tab:orange', label="Optimal $C_2$")

bbox = dict(boxstyle="round", fc="white")
ax.annotate(r'$C_{2|2}$', (0, C[1][1]), xytext=(-0.2, C[1][1]),
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)
ax.annotate(r'$C_{1|1}$', (1, C[0][0]), xytext=(1.1, C[0][0]),
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)
ax.annotate(r'$C_{1|2}$', (0, C[0][1]), xytext=(-0.2, C[0][1]),
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)
ax.annotate(r'$C_{2|1}$', (1, C[1][0]), xytext=(1.1, C[1][0]),
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)

ax.annotate(f'$t*={threshold:0.2}$', (threshold, cost_t),
            xytext=(threshold + 0.2, cost_t),
            arrowprops=dict(arrowstyle='->', facecolor='black'),
            bbox=bbox)

ax.set_xlabel('$P(C_1|x)$')
ax.set_ylabel('Expected cost')
ax.legend()

return fig
@output
@render.table(index=True)
def cost_matrix():
    global C_original
    C = C_original.T + input.S() # Need to transpose back to show print matrix
    C = C*fraction_to_float(input.M())

    return pd.DataFrame(C,
                        index=['True C1', 'True C2'],
                        columns=['Predicted C1', 'Predicted C2'])

app = App(app_ui, server, debug=True)

```

3.5.1 Simplification example

Because of these invariances, it is common in the binary case to modify the matrix c in such a way that the missclassification cost for one of the classes is 1 and a cost of 0 for its correct prediction. For example, if $c_{1|2}^* = 1$ and $c_{2|2}^* = 0$ we get

$$t^* = \frac{c_{1|2} - c_{2|2}}{c_{1|2} - c_{2|2} + c_{2|1} - c_{1|1}} = \frac{1}{1 + c_{2|1}^* - c_{1|1}^*} \quad (3.15)$$

In the previous example the original cost matrix c

$$c = \begin{bmatrix} -2 & 3 \\ 13 & -7 \end{bmatrix}^\top \quad (3.16)$$

if shifted by +7 and scaled by 1/20 results in

$$c' = \begin{bmatrix} (-2+7)/20 & (3+7)/20 \\ (13+7)/20 & (-7+7)/20 \end{bmatrix}^\top = \begin{bmatrix} 0.25 & 0.5 \\ 1 & 0 \end{bmatrix}^\top \quad (3.17)$$

with an optimal threshold

$$t^* = \frac{1}{1 + c_{2|1}' - c_{1|1}'} = \frac{1}{1 + 0.5 - 0.25} = 0.8 \quad (3.18)$$

3.6 Multiclass setting

The binary cost matrix can be extended to multiclass by extending the rows with additional true classes and columns with predicted classes.

	Predicted C_1	Predicted C_2	...	Predicted C_K
True C_1	$c_{1 1}$	$c_{2 1}$...	$c_{K 1}$
True C_2	$c_{1 2}$	$c_{2 2}$...	$c_{K 2}$
\vdots	\vdots	\vdots	\ddots	\vdots
True C_K	$c_{1 K}$	$c_{2 K}$...	$c_{K K}$

However, with more than 2 classes the threshold is not a single value but multiple decision boundaries in the probability simplex.

3.7 Ternary example {.smaller}

In order to exemplify the process of making an optimal decision in more with more than two classes we can look at the ternary case, which naturally extends to more classes. Given the following cost matrix

	Predicted C_1	Predicted C_2	Predicted C_3
True C_1	-10	20	30
True C_2	40	-50	60
True C_3	70	80	-90

and a true posterior probability vector for all the classes $[0.5, 0.1, 0.4]$, we can estimate the expected cost of making each class prediction

$$\mathbb{E}_{j \sim P(\cdot|\mathbf{x})}(c_{i|j}) = \sum_{j=1}^K P(C_j|\mathbf{x})c_{i|j}. \quad (3.19)$$

which results in the following expected costs:

- Predicting **Class 1** will have a cost of $-10 \times 0.5 + 40 \times 0.1 + 70 \times 0.4 = 27$
- Predicting **Class 2** will have a cost of $20 \times 0.5 - 50 \times 0.1 + 80 \times 0.4 = 37$
- Predicting **Class 3** will have a cost of $30 \times 0.5 + 60 \times 0.1 - 90 \times 0.4 = -15$

3.7.1 Ternary expected cost isolines per decision

```
import matplotlib.pyplot as plt
from pycalib.visualisations.barycentric import draw_func_contours

C = [[-10, 40, 70], [20, -50, 80], [30, 60, -90]]

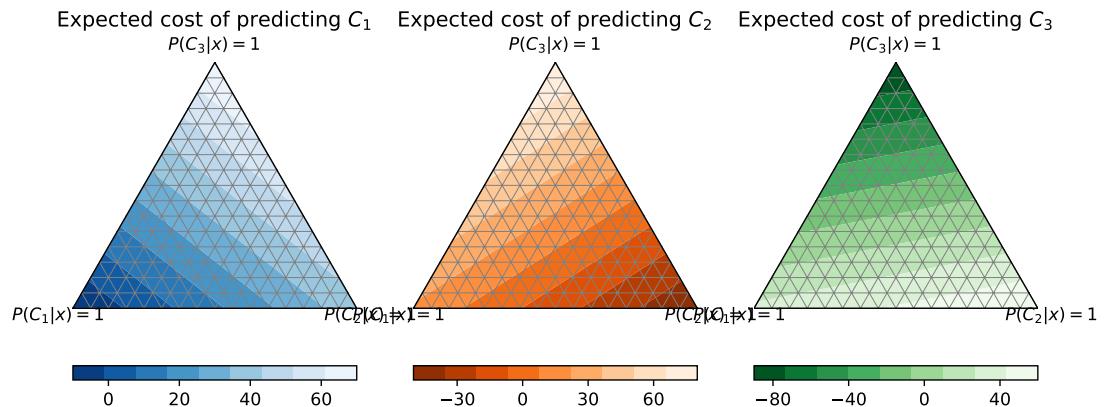
cmaps = ['Blues_r', 'Oranges_r', 'Greens_r']
labels = [f"$P(C_{i+1}|\mathbf{x}) = 1$" for i in range(len(C))]

fig = plt.figure(figsize=(10, 4))
for i in range(len(C)):
    ax = fig.add_subplot(1, len(C), i+1)
```

3 Cost-sensitive classification

```
def cost_func(prob):
    return sum(prob*C[i])

ax.set_title(f"Expected cost of predicting  $C_{i+1}$ ")
draw_func_contours(cost_func, labels=labels, nlevels=10, subdiv=4,
                  cmap=cmaps[i], fig=fig, ax=ax)
```



3.7.2 Ternary hyperplanes optimal decision combined

```
import matplotlib
import numpy as np
import matplotlib.pyplot as plt
from pycalib.visualisations.barycentric import draw_func_contours

C = [[-10, 40, 70], [20, -50, 80], [30, 60, -90]]

cmaps = ['Blues_r', 'Oranges_r', 'Greens_r']
labels = [f"$P(C_{i+1}|x) = 1$" for i in range(len(C))]

fig = plt.figure(figsize=(5, 5))
ax = fig.add_subplot()
fig.suptitle(f"Expected cost optimal prediction")
for i in range(len(C)):
    def cost_func(prob):
        expected_costs = np.inner(prob, C)
        min_p_id = np.argmin(expected_costs)
```

3.7 Ternary example {smaller}

```

if min_p_id == i:
    return expected_costs[i]
return np.nan

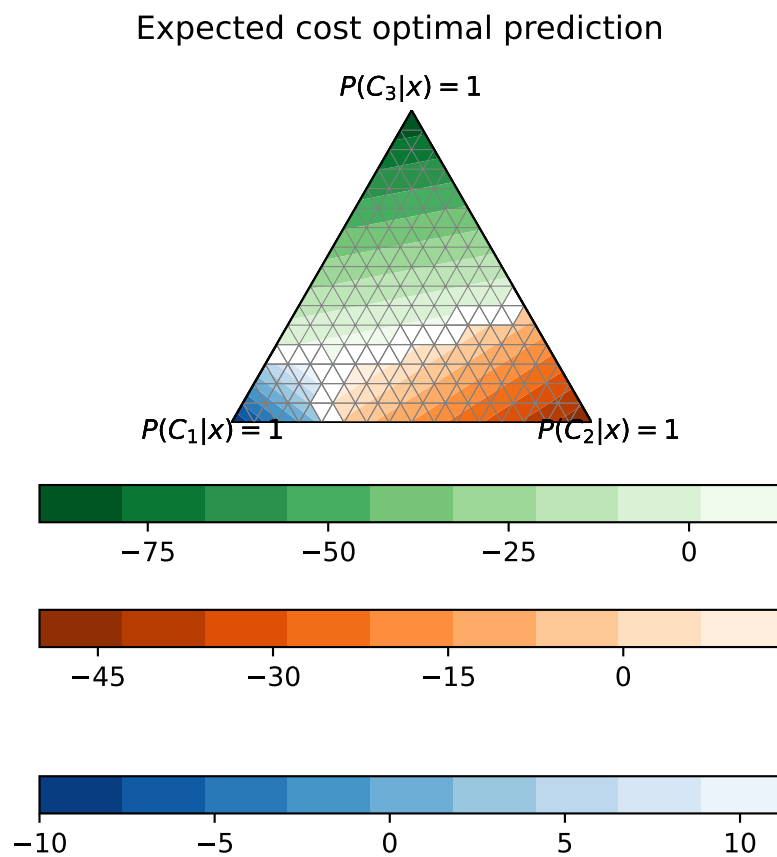
draw_func_contours(cost_func, labels=labels, nlevels=10, subdiv=4,
                   cmap=cmaps[i], cb_orientation='vertical', fig=fig, ax=ax)

plt.show()

```

/opt/hostedtoolcache/Python/3.10.14/x64/lib/python3.10/site-packages/pycalib/visualisations/ba

The following kwargs were not used by contour: 'cb_orientation'



3.8 Option to abstain

It is possible to add the costs of abstaining on making a prediction by adding a column into the original cost matrix [4]. The following is an example which illustrates this in a binary classification problem.

	Predicted C_1	Predicted C_2	Abstain
True C_1	0	10	2
True C_2	9	-3	2

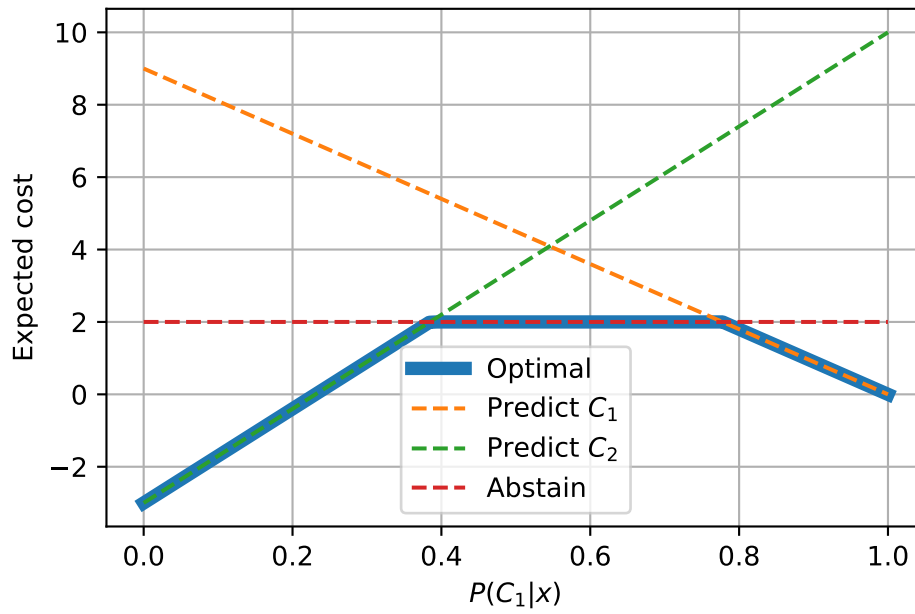
- Predicting **Class 1** has an expected cost of $0 \times 0.3 + 9 \times 0.7 = 6.3$
- Predicting **Class 2** has an expected cost of $10 \times 0.3 - 3 \times 0.7 = 0.9$
- **Abstaining** has an expected cost of $2 \times 0.3 + 2 \times 0.7 = 2$

3.8.1 Option to abstain cost lines

```
import numpy as np
import matplotlib.pyplot as plt

C = [[0, 9], [10, -3], [2, 2]]
p = np.linspace(0, 1, 100)
p = np.vstack([1 - p, p]).T
opt_cost = [min(np.inner(C, p[i])) for i in range(p.shape[0])]
plt.plot(p[:,0], opt_cost, lw=5, label='Optimal')

plt.grid(True)
plt.plot([0, 1], [C[0][1], C[0][0]], '--', label="Predict $C_1$")
plt.plot([0, 1], [C[1][1], C[1][0]], '--', label="Predict $C_2$")
plt.plot([0, 1], [C[2][1], C[2][0]], '--', c='tab:red', label="Abstain")
plt.xlabel('$P(C_1|x)$')
plt.ylabel('Expected cost')
plt.legend()
plt.show()
```

3.8.2 Option to abstain different costs

The following is another example in which abstaining from making a prediction if the true class was C_2 would incur into a gain.

	Predicted C_1	Predicted C_2	Abstain
True C_1	0	10	2
True C_2	9	-3	-1

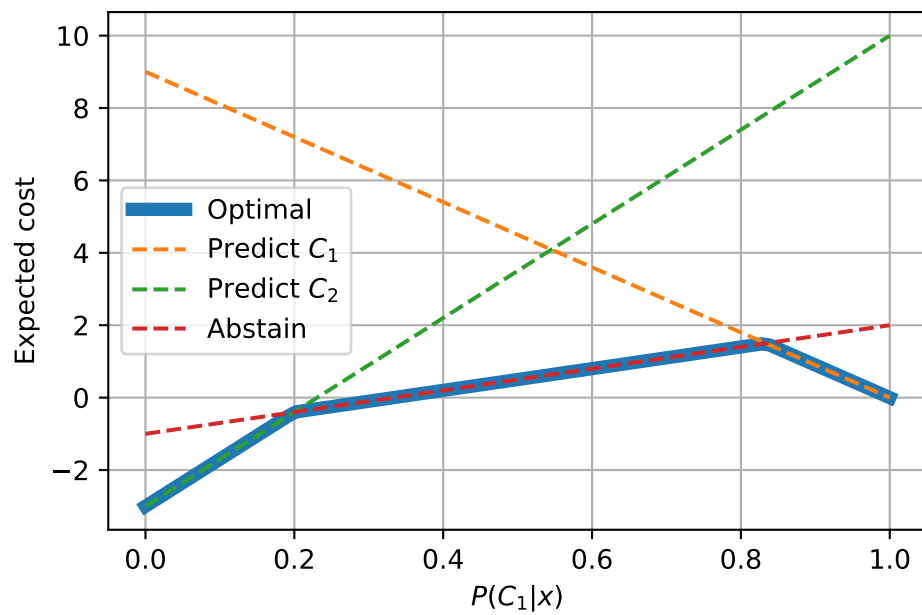
```
import numpy as np
import matplotlib.pyplot as plt

C = np.array([[0, 9], [10, -3], [2, -1]])
p = np.linspace(0, 1, 100)
p = np.vstack([1 - p, p]).T
opt_cost = [min(np.inner(C, p[i])) for i in range(p.shape[0])]
plt.plot(p[:,0], opt_cost, lw=5, label='Optimal')

plt.grid(True)
plt.plot([0, 1], [C[0][1], C[0][0]], '--', label="Predict $C_1$")
```

3 Cost-sensitive classification

```
plt.plot([0, 1], [C[1][1], C[1][0]], '--', label="Predict $C_2$")
plt.plot([0, 1], [C[2][1], C[2][0]], '--', c='tab:red', label="Abstain")
plt.xlabel('$P(C_1|x)$')
plt.ylabel('Expected cost')
plt.legend()
plt.show()
```



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