Machine Learning Homework 6

Environment

- Language: C++
- Standard: C++20

Code with detailed explanations

Libraries

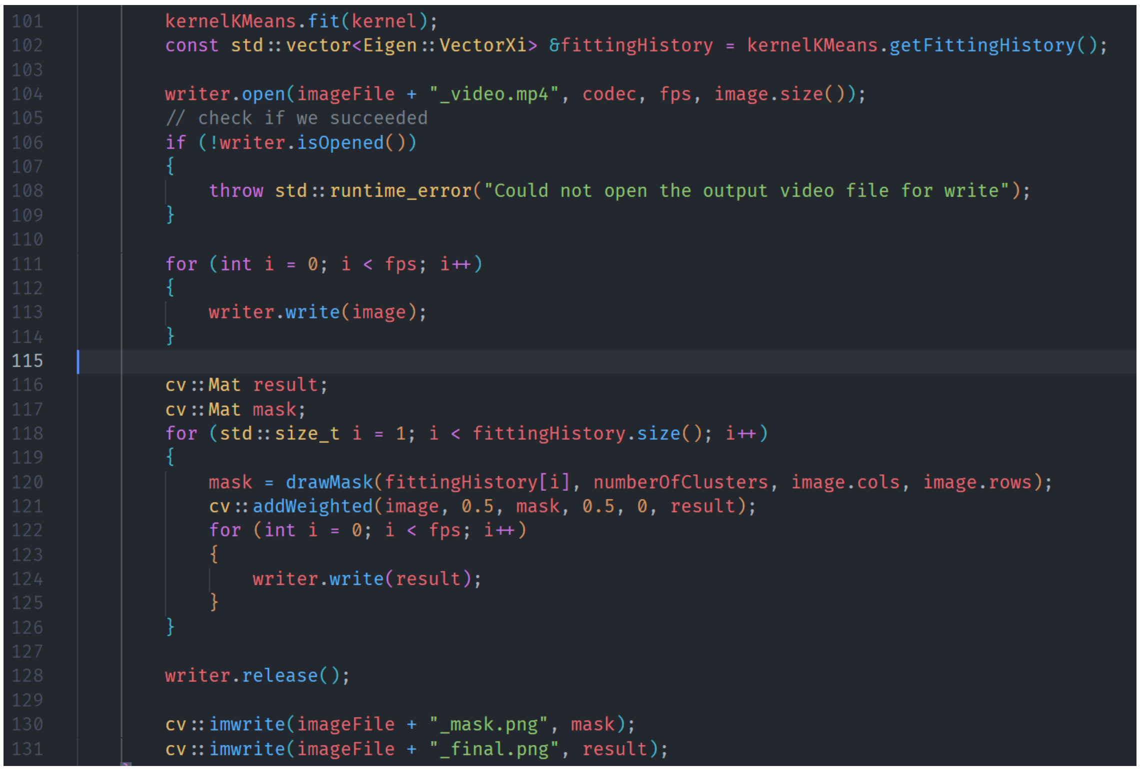
Used library => Corresponding library in homework description

- Eigen => numpy
- OpenCV, matplotlib++ => visualization
- Boost => filesystem, sort
- OpenMP (for parallel acceleration)

Visualization

- **Main part**

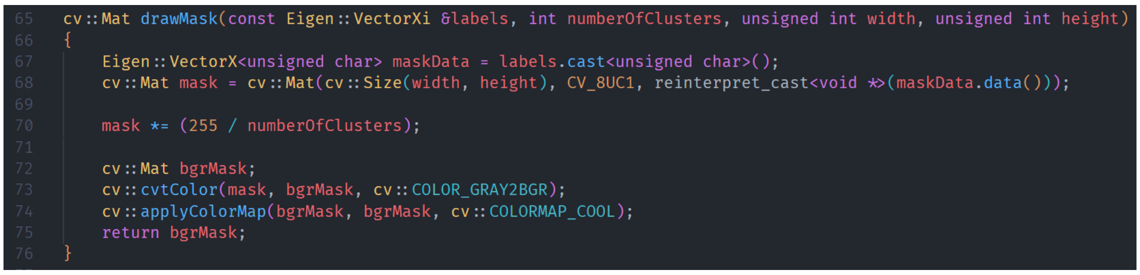
  > Use `fittingHistory` which records the labels for every iterations to make a video.
  >
  > The duration of one iteration is 1s.
  >
  > `cv::addWeighted` function is used to combine the clustering results (segmentation mask) with original image.
  >
  > `drawMask` function is used to convert the labels to segmentation mask.



```cpp
        kernelKMeans.fit(kernel);
        const std::vector<Eigen::VectorXi> &fittingHistory = kernelKMeans.getFittingHistory();

        writer.open(imageFile + "_video.mp4", codec, fps, image.size());
        // check if we succeeded
        if (!writer.isOpened())
        {
            throw std::runtime_error("Could not open the output video file for write");
        }

        for (int i = 0; i < fps; i++)
        {
            writer.write(image);
        }

        cv::Mat result;
        cv::Mat mask;
        for (std::size_t i = 1; i < fittingHistory.size(); i++)
        {
            mask = drawMask(fittingHistory[i], numberOfClusters, image.cols, image.rows);
            cv::addWeighted(image, 0.5, mask, 0.5, 0, result);
            for (int i = 0; i < fps; i++)
            {
                writer.write(result);
            }
        }

        writer.release();

        cv::imwrite(imageFile + "_mask.png", mask);
        cv::imwrite(imageFile + "_final.png", result);
```

- **Draw mask**

> Convert the labels to segmentation mask.
>
> `labels` contains the clustering results, from 0 to k-1.
>
> `cv::applyColorMap` is used to map the labels to the corresponding color to avoid duplicate colors.



```cpp
cv::Mat drawMask(const Eigen::VectorXi &labels, int numberOfClusters, unsigned int width, unsigned int height)
{
    Eigen::VectorX<unsigned char> maskData = labels.cast<unsigned char>();
    cv::Mat mask = cv::Mat(cv::Size(width, height), CV_8UC1, reinterpret_cast<void *>(maskData.data()));

    mask *= (255 / numberOfClusters);

    cv::Mat bgrMask;
    cv::cvtColor(mask, bgrMask, cv::COLOR_GRAY2BGR);
    cv::applyColorMap(bgrMask, bgrMask, cv::COLORMAP_COOL);
    return bgrMask;
}
```

Part1

- **Kernel K-Means**
    - Pseudo-code

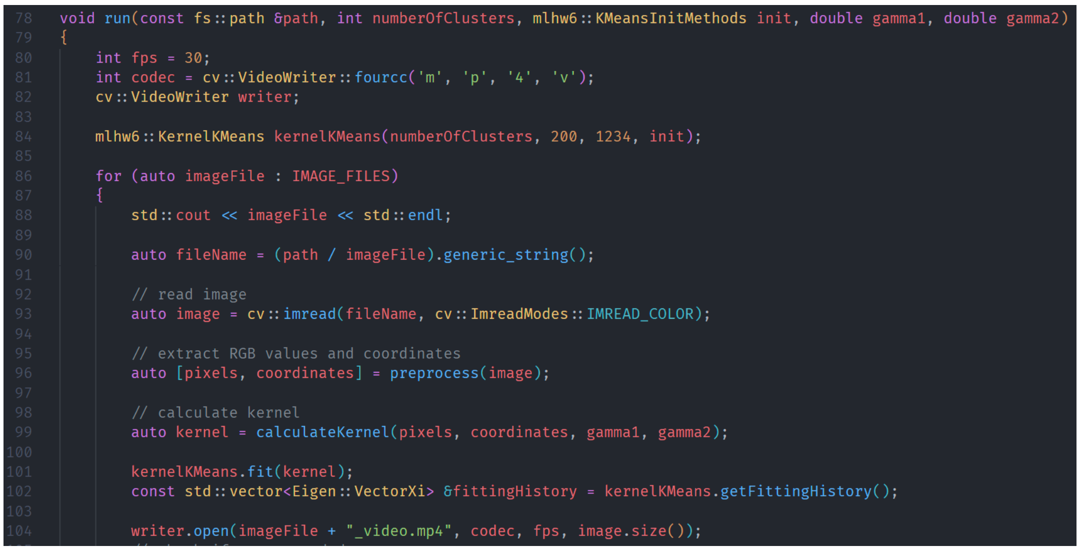
    > Ignore weight

ALGORITHM 1: Basic Batch Weighted Kernel k-means.

```
KERNEL_KMEANS_BATCH($K$, $k$, $w$, $t_{max}$, $\{\pi_c^{(0)}\}_{c=1}^k$, $\{\pi_c\}_{c=1}^k$)
Input: $K$: kernel matrix, $k$: number of clusters, $w$: weights for each point, $t_{max}$: optional maximum number of iterations, $\{\pi_c^{(0)}\}_{c=1}^k$: optional initial clusters
Output: $\{\pi_c\}_{c=1}^k$: final partitioning of the points
1. If no initial clustering is given, initialize the $k$ clusters $\pi_1^{(0)}, ..., \pi_k^{(0)}$ (i.e., randomly). Set $t = 0$.
2. For each point $\mathbf{a}_i$ and every cluster $c$, compute
       $$d(\mathbf{a}_i, \mathbf{m}_c) = K_{ii} - \frac{2\sum_{\mathbf{a}_j \in \pi_c^{(t)}} w_j K_{ij}}{\sum_{\mathbf{a}_j \in \pi_c^{(t)}} w_j} + \frac{\sum_{\mathbf{a}_j, \mathbf{a}_l \in \pi_c^{(t)}} w_j w_l K_{jl}}{(\sum_{\mathbf{a}_j \in \pi_c^{(t)}} w_j)^2}.$$
3. Find $c^*(\mathbf{a}_i) = \text{argmin}_c d(\mathbf{a}_i, \mathbf{m}_c)$, resolving ties arbitrarily. Compute the updated clusters as
       $$\pi_c^{(t+1)} = \{\mathbf{a} \ : \ c^*(\mathbf{a}_i) = c\}.$$
4. If not converged or $t_{max} > t$, set $t = t + 1$ and go to Step 2; Otherwise, stop and output final clusters $\{\pi_c^{(t+1)}\}_{c=1}^k$.
```

- Main function

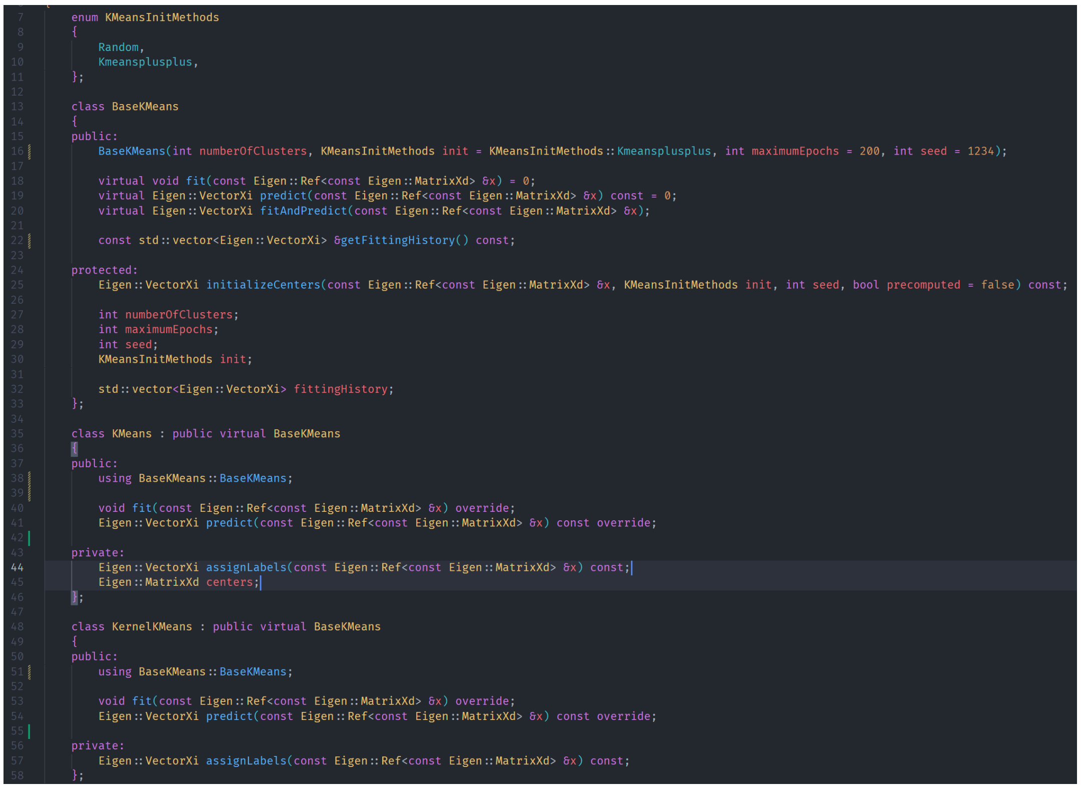
  > Arguments
  >
  > path: the image data folder
  >
  > numberOfClusters: the number of clusters
  >
  > init: the selected initialization method, random or k-means++
  >
  > gamma1, gamma2: the hyper-parameter of RBF kernel



```cpp
void run(const fs::path &path, int numberOfClusters, mlhw6::KMeansInitMethods init, double gamma1, double gamma2)
{
    int fps = 30;
    int codec = cv::VideoWriter::fourcc('m', 'p', '4', 'v');
    cv::VideoWriter writer;

    mlhw6::KernelKMeans kernelKMeans(numberOfClusters, 200, 1234, init);

    for (auto imageFile : IMAGE_FILES)
    {
        std::cout << imageFile << std::endl;

        auto fileName = (path / imageFile).generic_string();

        // read image
        auto image = cv::imread(fileName, cv::ImreadModes::IMREAD_COLOR);

        // extract RGB values and coordinates
        auto [pixels, coordinates] = preprocess(image);

        // calculate kernel
        auto kernel = calculateKernel(pixels, coordinates, gamma1, gamma2);

        kernelKMeans.fit(kernel);
        const std::vector<Eigen::VectorXi> &fittingHistory = kernelKMeans.getFittingHistory();

        writer.open(imageFile + "_video.mp4", codec, fps, image.size());
```

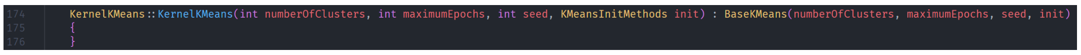
- `kmeans.h` header: k-means related classes

  > Follow the scikit-learn logic design.

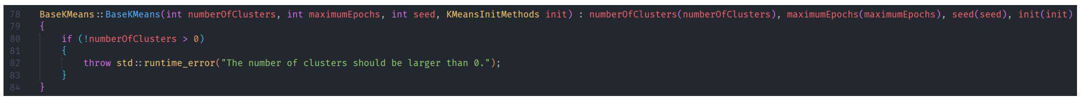


```cpp
    enum KMeansInitMethods
    {
        Random,
        Kmeansplusplus,
    };

    class BaseKMeans
    {
    public:
        BaseKMeans(int numberOfClusters, KMeansInitMethods init = KMeansInitMethods::Kmeansplusplus, int maximumEpochs = 200, int seed = 1234);

        virtual void fit(const Eigen::Ref<const Eigen::MatrixXd> &x) = 0;
        virtual Eigen::VectorXi predict(const Eigen::Ref<const Eigen::MatrixXd> &x) const = 0;
        virtual Eigen::VectorXi fitAndPredict(const Eigen::Ref<const Eigen::MatrixXd> &x);

        const std::vector<Eigen::VectorXi> &getFittingHistory() const;

    protected:
        Eigen::VectorXi initializeCenters(const Eigen::Ref<const Eigen::MatrixXd> &x, KMeansInitMethods init, int seed, bool precomputed = false) const;

        int numberOfClusters;
        int maximumEpochs;
        int seed;
        KMeansInitMethods init;

        std::vector<Eigen::VectorXi> fittingHistory;
    };

    class KMeans : public virtual BaseKMeans
    {
    public:
        using BaseKMeans::BaseKMeans;

        void fit(const Eigen::Ref<const Eigen::MatrixXd> &x) override;
        Eigen::VectorXi predict(const Eigen::Ref<const Eigen::MatrixXd> &x) const override;

    private:
        Eigen::VectorXi assignLabels(const Eigen::Ref<const Eigen::MatrixXd> &x) const;
        Eigen::MatrixXd centers;
    };

    class KernelKMeans : public virtual BaseKMeans
    {
    public:
        using BaseKMeans::BaseKMeans;

        void fit(const Eigen::Ref<const Eigen::MatrixXd> &x) override;
        Eigen::VectorXi predict(const Eigen::Ref<const Eigen::MatrixXd> &x) const override;

    private:
        Eigen::VectorXi assignLabels(const Eigen::Ref<const Eigen::MatrixXd> &x) const;
    };
```

- `KernelKMeans` constructor



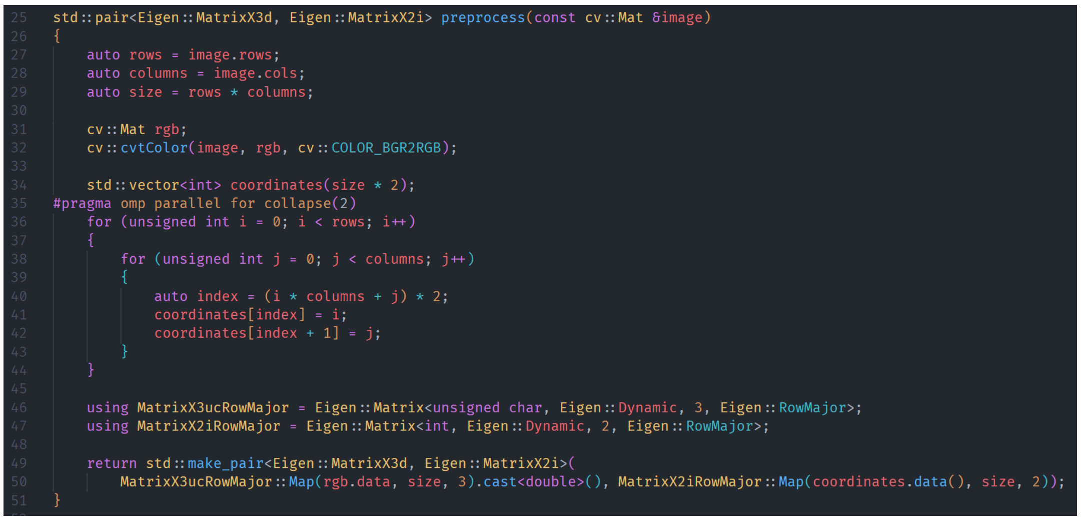
```cpp
    KernelKMeans::KernelKMeans(int numberOfClusters, int maximumEpochs, int seed, KMeansInitMethods init) : BaseKMeans(numberOfClusters, maximumEpochs, seed, init)
    {
    }
```



```cpp
BaseKMeans::BaseKMeans(int numberOfClusters, int maximumEpochs, int seed, KMeansInitMethods init) : numberOfClusters(numberOfClusters), maximumEpochs(maximumEpochs), seed(seed), init(init)
{
    if (!numberOfClusters > 0)
    {
        throw std::runtime_error("The number of clusters should be larger than 0.");
    }
}
```

- `preprocess` function: extract RGB values and coordinates

> Arguments
>
> image: (H, W, 3), BGR values



```cpp
std::pair<Eigen::MatrixX3d, Eigen::MatrixX2i> preprocess(const cv::Mat &image)
{
    auto rows = image.rows;
    auto columns = image.cols;
    auto size = rows * columns;

    cv::Mat rgb;
    cv::cvtColor(image, rgb, cv::COLOR_BGR2RGB);

    std::vector<int> coordinates(size * 2);
#pragma omp parallel for collapse(2)
    for (unsigned int i = 0; i < rows; i++)
    {
        for (unsigned int j = 0; j < columns; j++)
        {
            auto index = (i * columns + j) * 2;
            coordinates[index] = i;
            coordinates[index + 1] = j;
        }
    }

    using MatrixX3ucRowMajor = Eigen::Matrix<unsigned char, Eigen::Dynamic, 3, Eigen::RowMajor>;
    using MatrixX2iRowMajor = Eigen::Matrix<int, Eigen::Dynamic, 2, Eigen::RowMajor>;

    return std::make_pair<Eigen::MatrixX3d, Eigen::MatrixX2i>(
        MatrixX3ucRowMajor::Map(rgb.data, size, 3).cast<double>(), MatrixX2iRowMajor::Map(coordinates.data(), size, 2));
}
```

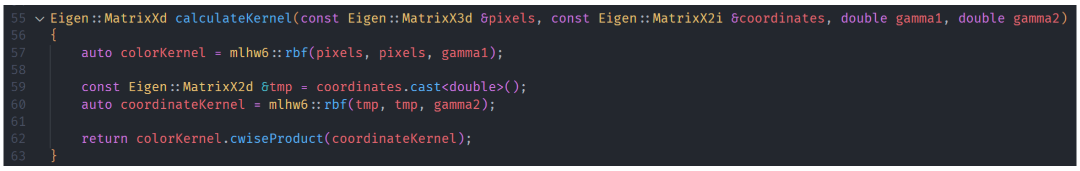
- `calculateKernel` function: calculate all kernel values

> Arguments
>
> pixels: (N, 3), RGB values
>
> coordinates: (N, 2), coordinates
>
> gamma1: γ_c scalar
>
> gamma2: γ_s scalar
>
> Formula

$$k(x, x') = e^{-\gamma_s \|S(x) - S(x')\|^2} \times e^{-\gamma_c \|C(x) - C(x')\|^2}$$

$S(x)$ is the spatial information (coordinate)

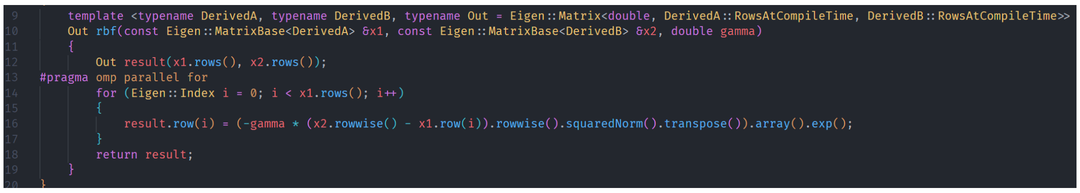
$C(x)$ is the color information (RGB)



```cpp
Eigen::MatrixXd calculateKernel(const Eigen::MatrixX3d &pixels, const Eigen::MatrixX2i &coordinates, double gamma1, double gamma2)
{
    auto colorKernel = mlhw6::rbf(pixels, pixels, gamma1);

    const Eigen::MatrixX2d &tmp = coordinates.cast<double>();
    auto coordinateKernel = mlhw6::rbf(tmp, tmp, gamma2);

    return colorKernel.cwiseProduct(coordinateKernel);
}
```

- `rbf` function: RBF kernel

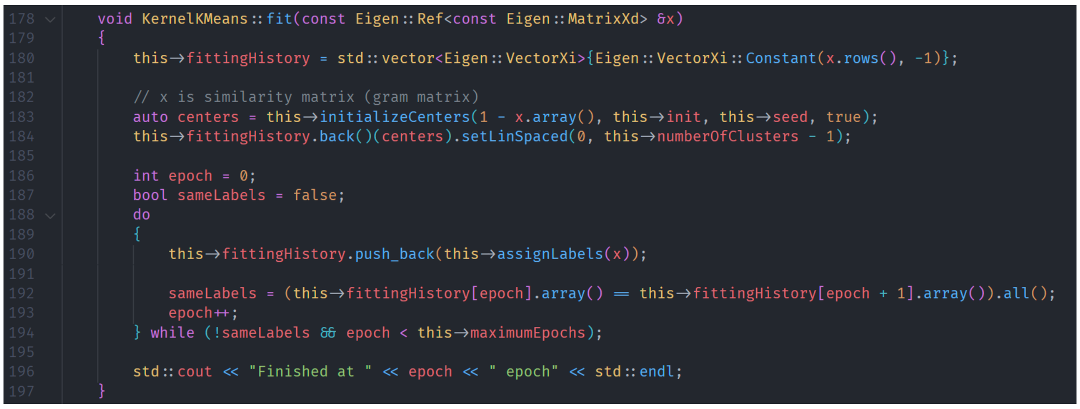
> Arguments
>
> x1: x vector
>
> x2: x' vector
>
> gamma: γ scalar
>
> Formula
>
> $k(x, x') = e^{-\gamma||x-x'||^2}$



```cpp
    template <typename DerivedA, typename DerivedB, typename Out = Eigen::Matrix<double, DerivedA::RowsAtCompileTime, DerivedB::RowsAtCompileTime>>
    Out rbf(const Eigen::MatrixBase<DerivedA> &x1, const Eigen::MatrixBase<DerivedB> &x2, double gamma)
    {
        Out result(x1.rows(), x2.rows());
#pragma omp parallel for
        for (Eigen::Index i = 0; i < x1.rows(); i++)
        {
            result.row(i) = (-gamma * (x2.rowwise() - x1.row(i)).rowwise().squaredNorm().transpose()).array().exp();
        }
        return result;
    }
}
```

- `kernelKMeans.fit` function: fit the data

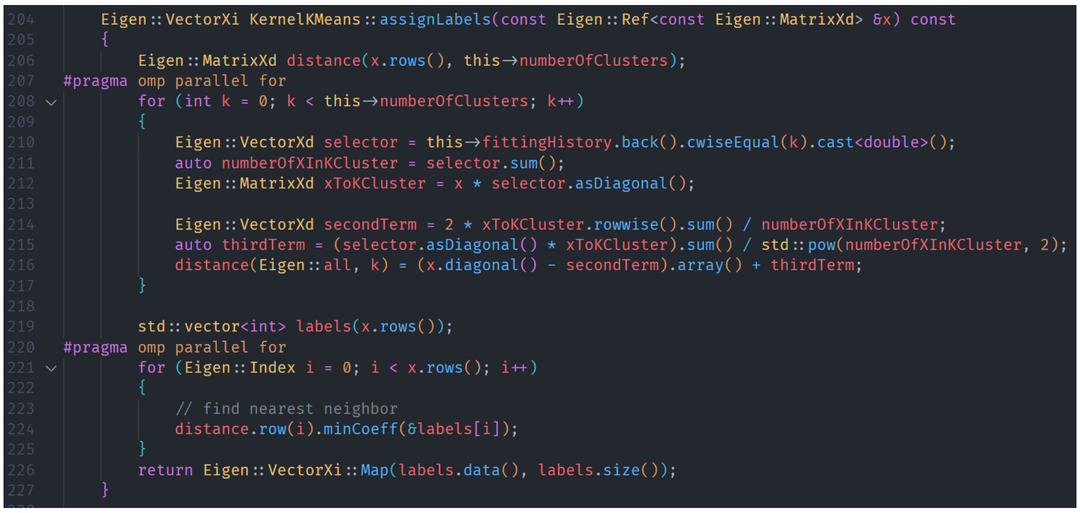
> Previously, we already calculated the kernel.
>
> So, we use the precomputed kernel values directly.
>
> Arguments
>
> x: (N, N), the kernel values (gram matrix, similarity matrix)
>
> Steps
>
> 1. Pick k centers
> 2. Calculate the cost between the data and centers
> 3. Assign the label which has the smallest distance to the data
> 4. Keep repeating 2, 3 step until the labels are not changed
>
> `fittingHistory` is used to store the labels for every iterations.
>
> Note: At the line 183, we do $1 - x$ to get the distance matrix.



```cpp
178     void KernelKMeans::fit(const Eigen::Ref<const Eigen::MatrixXd> &x)
179     {
180         this->fittingHistory = std::vector<Eigen::VectorXi>{Eigen::VectorXi::Constant(x.rows(), -1)};
181 
182         // x is similarity matrix (gram matrix)
183         auto centers = this->initializeCenters(1 - x.array(), this->init, this->seed, true);
184         this->fittingHistory.back()(centers).setLinSpaced(0, this->numberOfClusters - 1);
185 
186         int epoch = 0;
187         bool sameLabels = false;
188         do
189         {
190             this->fittingHistory.push_back(this->assignLabels(x));
191 
192             sameLabels = (this->fittingHistory[epoch].array() == this->fittingHistory[epoch + 1].array()).all();
193             epoch++;
194         } while (!sameLabels && epoch < this->maximumEpochs);
195 
196         std::cout << "Finished at " << epoch << " epoch" << std::endl;
197     }
```

- `assignLabels` function: calculate the cost and assign labels

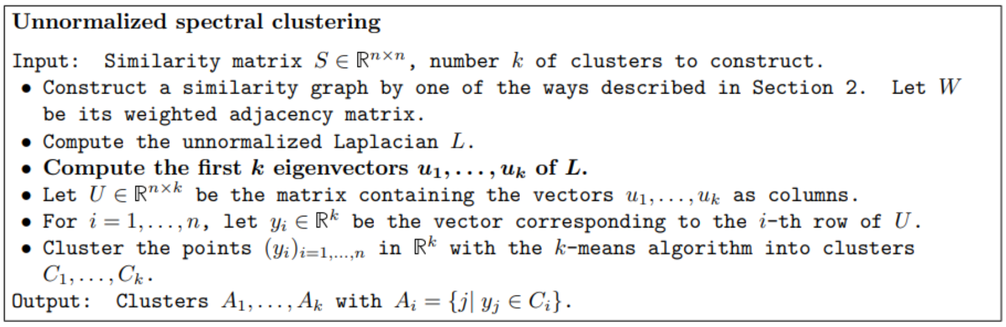
  > Arguments
  >
  > x: (N, N), the kernel values
  >
  > Steps
  >
  > 1. Calculate the cost between the data and centers
  >
  > $$\mathbf{k}(x_j, x_j) - \frac{2}{|C_k|}\sum_n \alpha_{kn}\mathbf{k}(x_j, x_n) + \frac{1}{|C_k|^2}\sum_p\sum_q \alpha_{kp}\alpha_{kq}\mathbf{k}(x_p, x_q)$$
  >
  > 2. Assign the label which has the smallest distance to the data



```cpp
    Eigen::VectorXi KernelKMeans::assignLabels(const Eigen::Ref<const Eigen::MatrixXd> &x) const
    {
        Eigen::MatrixXd distance(x.rows(), this->numberOfClusters);
#pragma omp parallel for
        for (int k = 0; k < this->numberOfClusters; k++)
        {
            Eigen::VectorXd selector = this->fittingHistory.back().cwiseEqual(k).cast<double>();
            auto numberOfXInKCluster = selector.sum();
            Eigen::MatrixXd xToKCluster = x * selector.asDiagonal();

            Eigen::VectorXd secondTerm = 2 * xToKCluster.rowwise().sum() / numberOfXInKCluster;
            auto thirdTerm = (selector.asDiagonal() * xToKCluster).sum() / std::pow(numberOfXInKCluster, 2);
            distance(Eigen::all, k) = (x.diagonal() - secondTerm).array() + thirdTerm;
        }

        std::vector<int> labels(x.rows());
#pragma omp parallel for
        for (Eigen::Index i = 0; i < x.rows(); i++)
        {
            // find nearest neighbor
            distance.row(i).minCoeff(&labels[i]);
        }
        return Eigen::VectorXi::Map(labels.data(), labels.size());
    }
```

Spectral Clustering

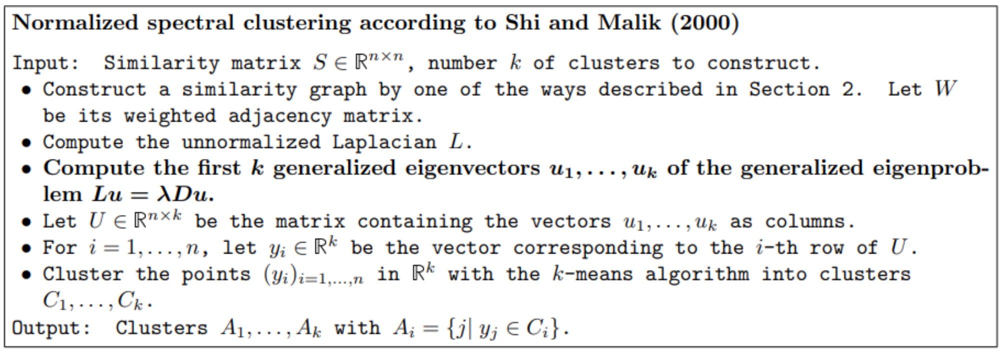
- Pseudo-code
  - Spectral Clustering (ratio cut)



Unnormalized spectral clustering

```
Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number $k$ of clusters to construct.
  • Construct a similarity graph by one of the ways described in Section 2. Let $W$
    be its weighted adjacency matrix.
  • Compute the unnormalized Laplacian $L$.
  • Compute the first $k$ eigenvectors $u_1, \dots, u_k$ of $L$.
  • Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors $u_1, \dots, u_k$ as columns.
  • For $i = 1, \dots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the $i$-th row of $U$.
  • Cluster the points $(y_i)_{i=1,\dots,n}$ in $\mathbb{R}^k$ with the $k$-means algorithm into clusters
    $C_1, \dots, C_k$.
Output: Clusters $A_1, \dots, A_k$ with $A_i = \{j | y_j \in C_i\}$.
```

  - Normalized Spectral Clustering (normalized cut)



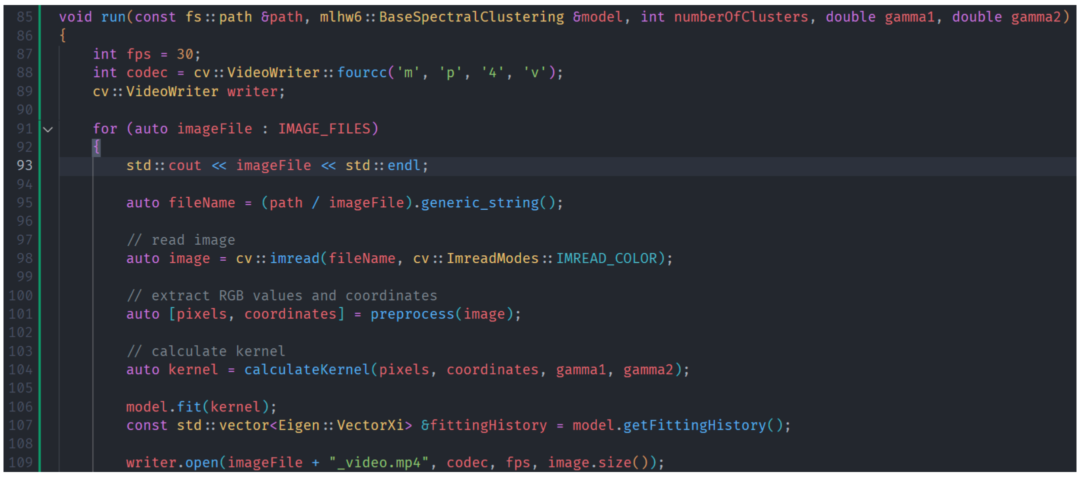
Normalized spectral clustering according to Shi and Malik (2000)

```
Input: Similarity matrix $S \in \mathbb{R}^{n \times n}$, number $k$ of clusters to construct.
  • Construct a similarity graph by one of the ways described in Section 2. Let $W$
    be its weighted adjacency matrix.
  • Compute the unnormalized Laplacian $L$.
  • Compute the first $k$ generalized eigenvectors $u_1, \dots, u_k$ of the generalized eigenprob-
    lem $Lu = \lambda Du$.
  • Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors $u_1, \dots, u_k$ as columns.
  • For $i = 1, \dots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the $i$-th row of $U$.
  • Cluster the points $(y_i)_{i=1,\dots,n}$ in $\mathbb{R}^k$ with the $k$-means algorithm into clusters
    $C_1, \dots, C_k$.
Output: Clusters $A_1, \dots, A_k$ with $A_i = \{j | y_j \in C_i\}$.
```

- Main function

> Arguments
>
> path: the image data folder
>
> model: Spectral Clustering instance
>
> numberOfClusters: the number of clusters
>
> gamma1, gamma2: the hyper-parameter of RBF kernel

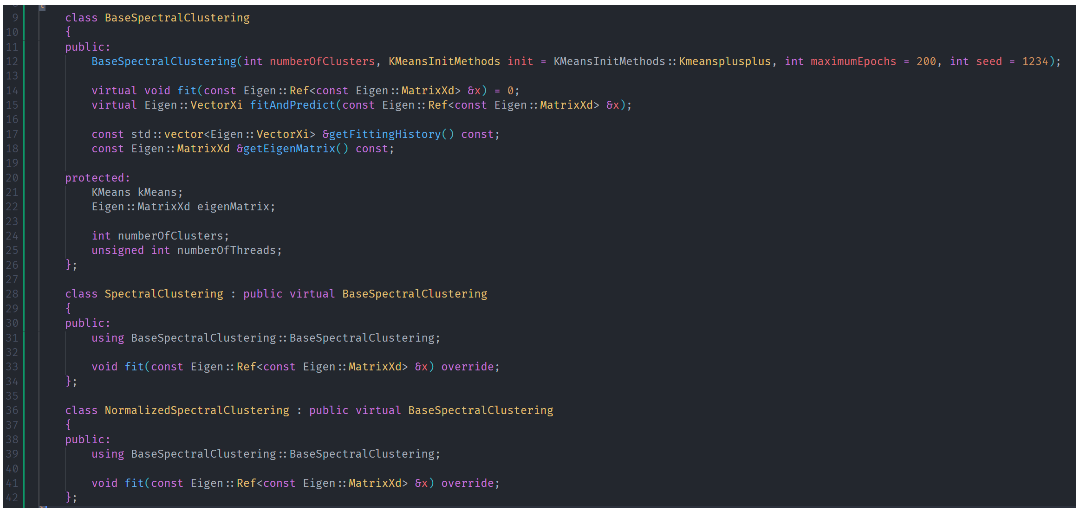
```cpp
switch (type)
{
case SpectralClusteringType::Unnormalized:
{
    auto model = mlhw6::SpectralClustering(numberOfClusters, init);
    run(path, model, numberOfClusters, gamma1, gamma2);
    break;
}
case SpectralClusteringType::Normalized:
{
    auto model = mlhw6::NormalizedSpectralClustering(numberOfClusters, init);
    run(path, model, numberOfClusters, gamma1, gamma2);
    break;
}
default:
    std::cerr << "Unknown spectral clustering type." << std::endl;
    return 1;
}
```



```cpp
void run(const fs::path &path, mlhw6::BaseSpectralClustering &model, int numberOfClusters, double gamma1, double gamma2)
{
    int fps = 30;
    int codec = cv::VideoWriter::fourcc('m', 'p', '4', 'v');
    cv::VideoWriter writer;

    for (auto imageFile : IMAGE_FILES)
    {
        std::cout << imageFile << std::endl;

        auto fileName = (path / imageFile).generic_string();

        // read image
        auto image = cv::imread(fileName, cv::ImreadModes::IMREAD_COLOR);

        // extract RGB values and coordinates
        auto [pixels, coordinates] = preprocess(image);

        // calculate kernel
        auto kernel = calculateKernel(pixels, coordinates, gamma1, gamma2);

        model.fit(kernel);
        const std::vector<Eigen::VectorXi> &fittingHistory = model.getFittingHistory();

        writer.open(imageFile + "_video.mp4", codec, fps, image.size());
```

- `spectral.h` header: spectral clustering related classes

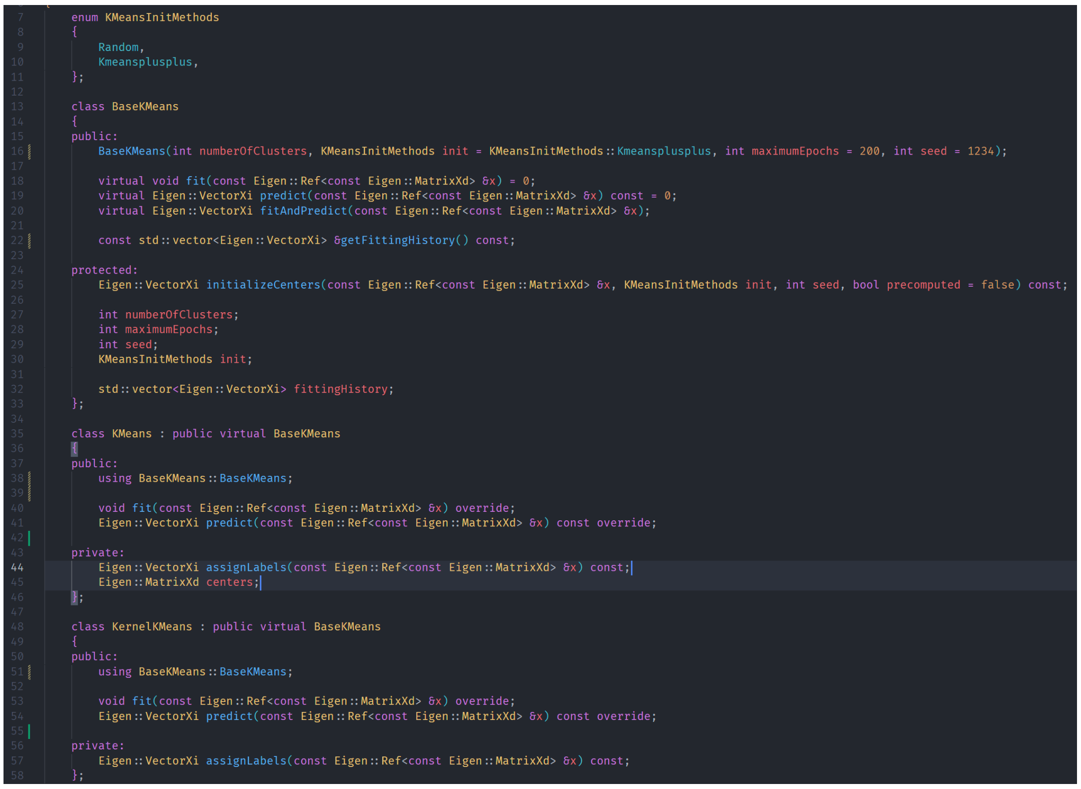
  > Follow the scikit-learn logic design.



```cpp
class BaseSpectralClustering
{
public:
    BaseSpectralClustering(int numberOfClusters, KMeansInitMethods init = KMeansInitMethods::Kmeansplusplus, int maximumEpochs = 200, int seed = 1234);

    virtual void fit(const Eigen::Ref<const Eigen::MatrixXd> &x) = 0;
    virtual Eigen::VectorXi fitAndPredict(const Eigen::Ref<const Eigen::MatrixXd> &x);

    const std::vector<Eigen::VectorXi> &getFittingHistory() const;
    const Eigen::MatrixXd &getEigenMatrix() const;

protected:
    KMeans kMeans;
    Eigen::MatrixXd eigenMatrix;

    int numberOfClusters;
    unsigned int numberOfThreads;
};

class SpectralClustering : public virtual BaseSpectralClustering
{
public:
    using BaseSpectralClustering::BaseSpectralClustering;

    void fit(const Eigen::Ref<const Eigen::MatrixXd> &x) override;
};

class NormalizedSpectralClustering : public virtual BaseSpectralClustering
{
public:
    using BaseSpectralClustering::BaseSpectralClustering;

    void fit(const Eigen::Ref<const Eigen::MatrixXd> &x) override;
};
```

- `kmeans.h` header: k-means related classes

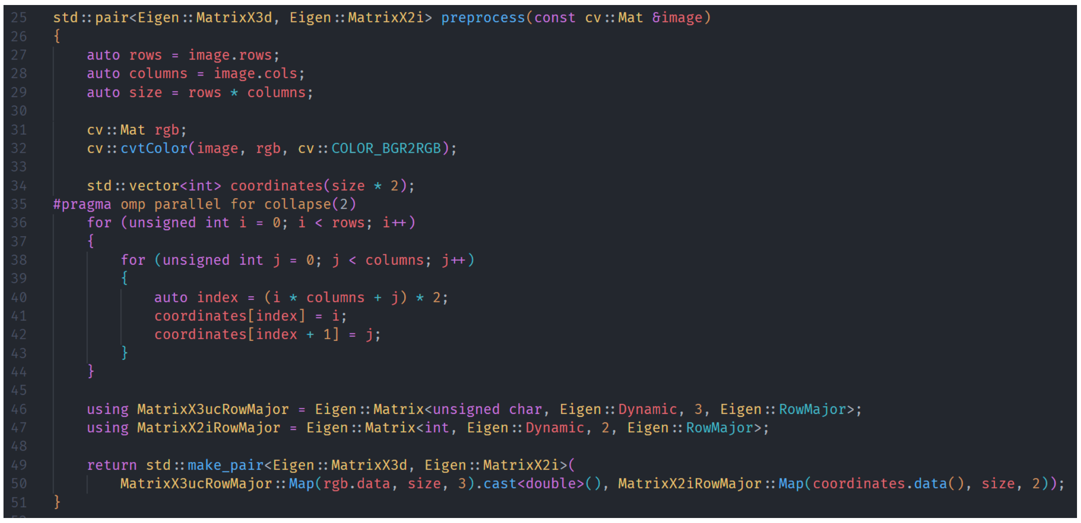
  > Follow the scikit-learn logic design.



```cpp
    enum KMeansInitMethods
    {
        Random,
        Kmeansplusplus,
    };

    class BaseKMeans
    {
    public:
        BaseKMeans(int numberOfClusters, KMeansInitMethods init = KMeansInitMethods::Kmeansplusplus, int maximumEpochs = 200, int seed = 1234);

        virtual void fit(const Eigen::Ref<const Eigen::MatrixXd> &x) = 0;
        virtual Eigen::VectorXi predict(const Eigen::Ref<const Eigen::MatrixXd> &x) const = 0;
        virtual Eigen::VectorXi fitAndPredict(const Eigen::Ref<const Eigen::MatrixXd> &x);

        const std::vector<Eigen::VectorXi> &getFittingHistory() const;

    protected:
        Eigen::VectorXi initializeCenters(const Eigen::Ref<const Eigen::MatrixXd> &x, KMeansInitMethods init, int seed, bool precomputed = false) const;

        int numberOfClusters;
        int maximumEpochs;
        int seed;
        KMeansInitMethods init;

        std::vector<Eigen::VectorXi> fittingHistory;
    };

    class KMeans : public virtual BaseKMeans
    {
    public:
        using BaseKMeans::BaseKMeans;

        void fit(const Eigen::Ref<const Eigen::MatrixXd> &x) override;
        Eigen::VectorXi predict(const Eigen::Ref<const Eigen::MatrixXd> &x) const override;

    private:
        Eigen::VectorXi assignLabels(const Eigen::Ref<const Eigen::MatrixXd> &x) const;
        Eigen::MatrixXd centers;
    };

    class KernelKMeans : public virtual BaseKMeans
    {
    public:
        using BaseKMeans::BaseKMeans;

        void fit(const Eigen::Ref<const Eigen::MatrixXd> &x) override;
        Eigen::VectorXi predict(const Eigen::Ref<const Eigen::MatrixXd> &x) const override;

    private:
        Eigen::VectorXi assignLabels(const Eigen::Ref<const Eigen::MatrixXd> &x) const;
    };
```

- `preprocess` function: extract RGB values and coordinates

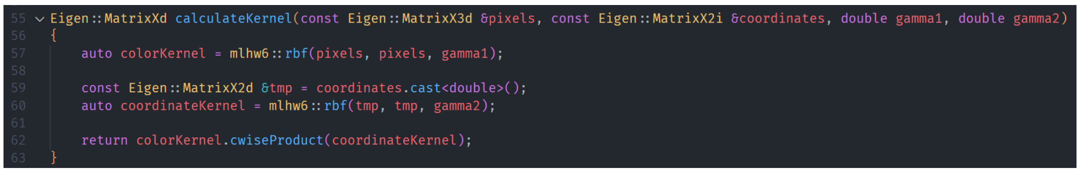
> Arguments
>
> image: (H, W, 3), BGR values



```cpp
std::pair<Eigen::MatrixX3d, Eigen::MatrixX2i> preprocess(const cv::Mat &image)
{
    auto rows = image.rows;
    auto columns = image.cols;
    auto size = rows * columns;

    cv::Mat rgb;
    cv::cvtColor(image, rgb, cv::COLOR_BGR2RGB);

    std::vector<int> coordinates(size * 2);
#pragma omp parallel for collapse(2)
    for (unsigned int i = 0; i < rows; i++)
    {
        for (unsigned int j = 0; j < columns; j++)
        {
            auto index = (i * columns + j) * 2;
            coordinates[index] = i;
            coordinates[index + 1] = j;
        }
    }

    using MatrixX3ucRowMajor = Eigen::Matrix<unsigned char, Eigen::Dynamic, 3, Eigen::RowMajor>;
    using MatrixX2iRowMajor = Eigen::Matrix<int, Eigen::Dynamic, 2, Eigen::RowMajor>;

    return std::make_pair<Eigen::MatrixX3d, Eigen::MatrixX2i>(
        MatrixX3ucRowMajor::Map(rgb.data, size, 3).cast<double>(), MatrixX2iRowMajor::Map(coordinates.data(), size, 2));
}
```

- `calculateKernel` function: calculate all kernel values

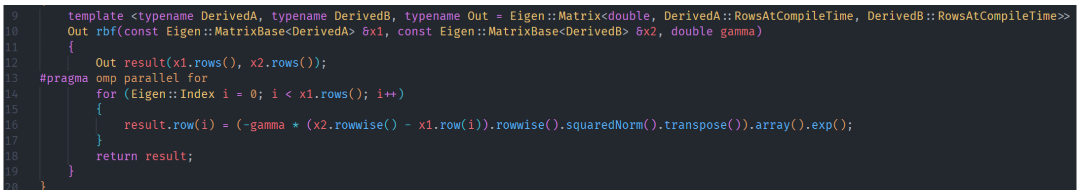
> Arguments
>
> pixels: (N, 3), RGB values
>
> coordinates: (N, 2), coordinates
>
> gamma1: γ_c scalar
>
> gamma2: γ_s scalar
>
> Formula
>
> $$k(x, x') = e^{-\gamma_s \|S(x)-S(x')\|^2} \times e^{-\gamma_c \|C(x)-C(x')\|^2}$$
>
> $S(x)$ is the spatial information (coordinate)
>
> $C(x)$ is the color information (RGB)



```cpp
Eigen::MatrixXd calculateKernel(const Eigen::MatrixX3d &pixels, const Eigen::MatrixX2i &coordinates, double gamma1, double gamma2)
{
    auto colorKernel = mlhw6::rbf(pixels, pixels, gamma1);

    const Eigen::MatrixX2d &tmp = coordinates.cast<double>();
    auto coordinateKernel = mlhw6::rbf(tmp, tmp, gamma2);

    return colorKernel.cwiseProduct(coordinateKernel);
}
```

- `rbf` function: RBF kernel

  > Arguments
  >
  > x1: x vector
  >
  > x2: x' vector
  >
  > gamma: γ scalar
  >
  > Formula
  >
  > $$k(x, x') = e^{-\gamma||x-x'||^2}$$



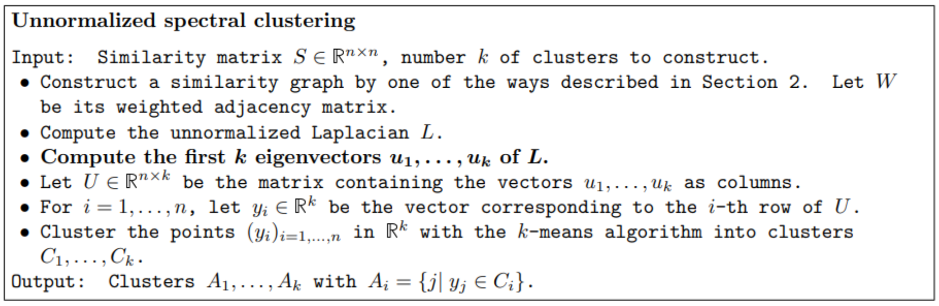
```cpp
    template <typename DerivedA, typename DerivedB, typename Out = Eigen::Matrix<double, DerivedA::RowsAtCompileTime, DerivedB::RowsAtCompileTime>>
    Out rbf(const Eigen::MatrixBase<DerivedA> &x1, const Eigen::MatrixBase<DerivedB> &x2, double gamma)
    {
        Out result(x1.rows(), x2.rows());
#pragma omp parallel for
        for (Eigen::Index i = 0; i < x1.rows(); i++)
        {
            result.row(i) = (-gamma * (x2.rowwise() - x1.row(i)).rowwise().squaredNorm().transpose()).array().exp();
        }
        return result;
    }
}
```

- `model.fit` function: fit the data

  > Previously, we already calculated the kernel.
  >
  > So, we use the precomputed kernel values directly.
  >
  > Arguments
  >
  > x: (N, N), the kernel values (gram matrix, similarity matrix)

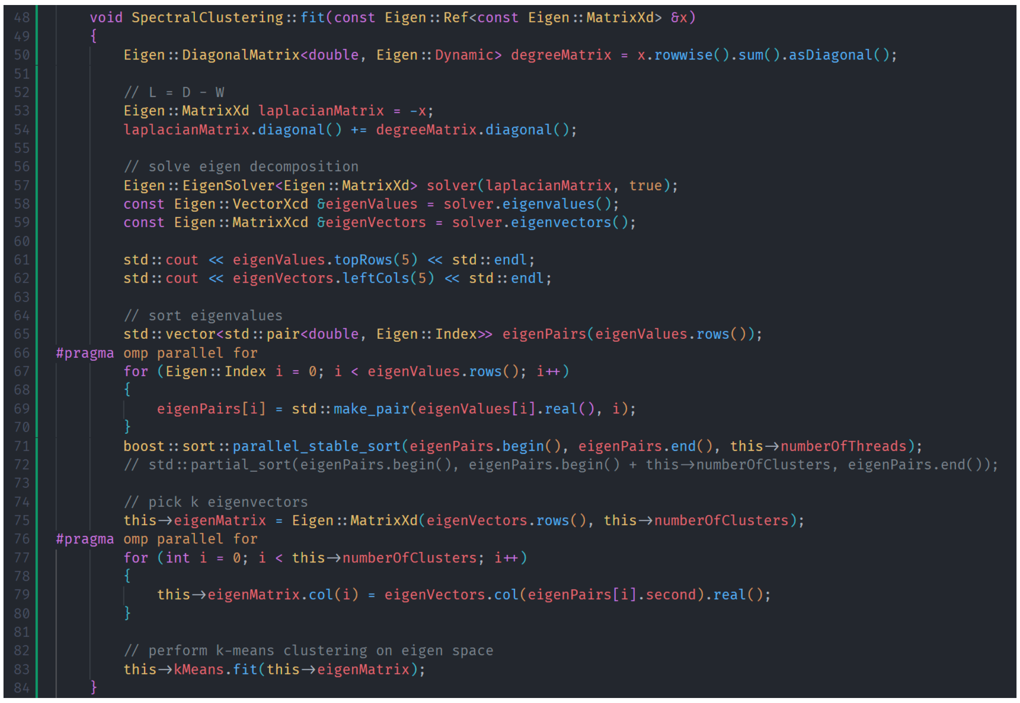
  - Spectral Clustering (ratio cut)

    > Algorithm



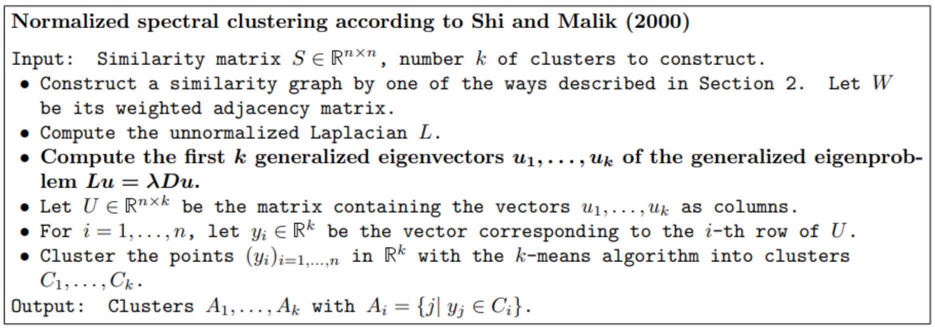
Unnormalized spectral clustering

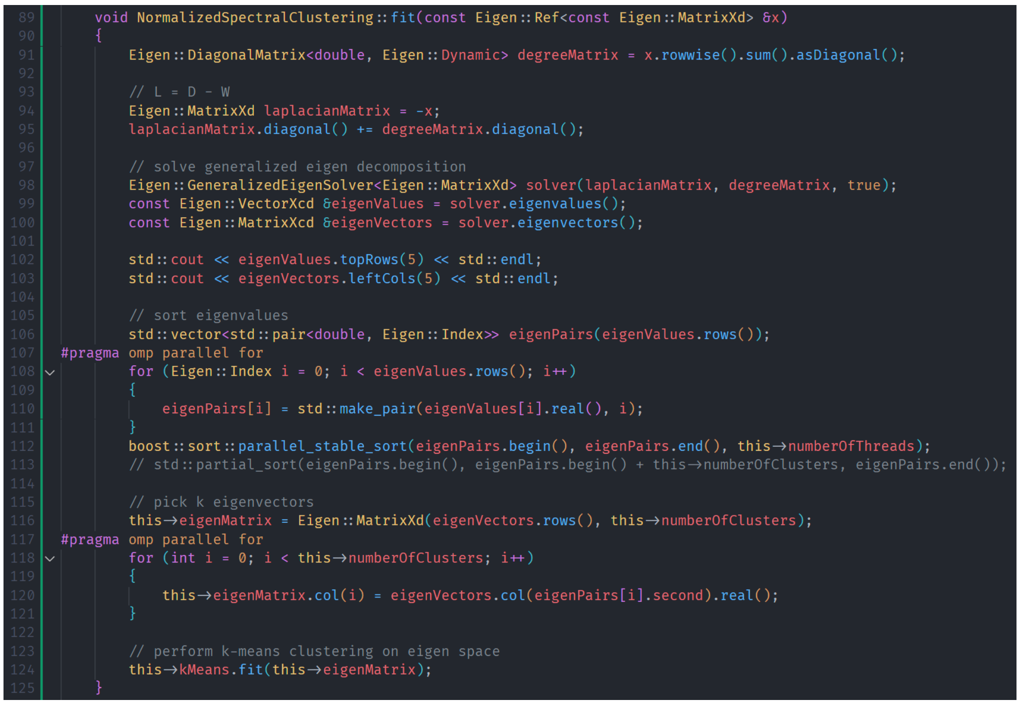
```
Input:  Similarity matrix $S \in \mathbb{R}^{n \times n}$, number $k$ of clusters to construct.
  • Construct a similarity graph by one of the ways described in Section 2.  Let $W$
    be its weighted adjacency matrix.
  • Compute the unnormalized Laplacian $L$.
  • Compute the first $k$ eigenvectors $u_1, \ldots, u_k$ of $L$.
  • Let $U \in \mathbb{R}^{n \times k}$ be the matrix containing the vectors $u_1, \ldots, u_k$ as columns.
  • For $i = 1, \ldots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the $i$-th row of $U$.
  • Cluster the points $(y_i)_{i=1,\ldots,n}$ in $\mathbb{R}^k$ with the $k$-means algorithm into clusters
    $C_1, \ldots, C_k$.
Output:  Clusters $A_1, \ldots, A_k$ with $A_i = \{j | y_j \in C_i\}$.
```



```cpp
    void SpectralClustering::fit(const Eigen::Ref<const Eigen::MatrixXd> &x)
    {
        Eigen::DiagonalMatrix<double, Eigen::Dynamic> degreeMatrix = x.rowwise().sum().asDiagonal();

        // L = D - W
        Eigen::MatrixXd laplacianMatrix = -x;
        laplacianMatrix.diagonal() += degreeMatrix.diagonal();

        // solve eigen decomposition
        Eigen::EigenSolver<Eigen::MatrixXd> solver(laplacianMatrix, true);
        const Eigen::VectorXcd &eigenValues = solver.eigenvalues();
        const Eigen::MatrixXcd &eigenVectors = solver.eigenvectors();

        std::cout << eigenValues.topRows(5) << std::endl;
        std::cout << eigenVectors.leftCols(5) << std::endl;

        // sort eigenvalues
        std::vector<std::pair<double, Eigen::Index>> eigenPairs(eigenValues.rows());
#pragma omp parallel for
        for (Eigen::Index i = 0; i < eigenValues.rows(); i++)
        {
            eigenPairs[i] = std::make_pair(eigenValues[i].real(), i);
        }
        boost::sort::parallel_stable_sort(eigenPairs.begin(), eigenPairs.end(), this->numberOfThreads);
        // std::partial_sort(eigenPairs.begin(), eigenPairs.begin() + this->numberOfClusters, eigenPairs.end());

        // pick k eigenvectors
        this->eigenMatrix = Eigen::MatrixXd(eigenVectors.rows(), this->numberOfClusters);
#pragma omp parallel for
        for (int i = 0; i < this->numberOfClusters; i++)
        {
            this->eigenMatrix.col(i) = eigenVectors.col(eigenPairs[i].second).real();
        }

        // perform k-means clustering on eigen space
        this->kMeans.fit(this->eigenMatrix);
    }
```

- Normalized Spectral Clustering (normalized cut)

> Algorithm
>
> 
>
> **Normalized spectral clustering according to Shi and Malik (2000)**
>
> Input: Similarity matrix $S \in \mathbb{R}^{n\times n}$, number k of clusters to construct.
> - Construct a similarity graph by one of the ways described in Section 2. Let W be its weighted adjacency matrix.
> - Compute the unnormalized Laplacian L.
> - **Compute the first k generalized eigenvectors $u_1, \dots, u_k$ of the generalized eigenproblem $Lu = \lambda Du$.**
> - Let $U \in \mathbb{R}^{n\times k}$ be the matrix containing the vectors $u_1, \dots, u_k$ as columns.
> - For $i = 1, \dots, n$, let $y_i \in \mathbb{R}^k$ be the vector corresponding to the i-th row of U.
> - Cluster the points $(y_i)_{i=1,\dots,n}$ in $\mathbb{R}^k$ with the k-means algorithm into clusters $C_1, \dots, C_k$.
>
> Output: Clusters $A_1, \dots, A_k$ with $A_i = \{j \mid y_j \in C_i\}$.

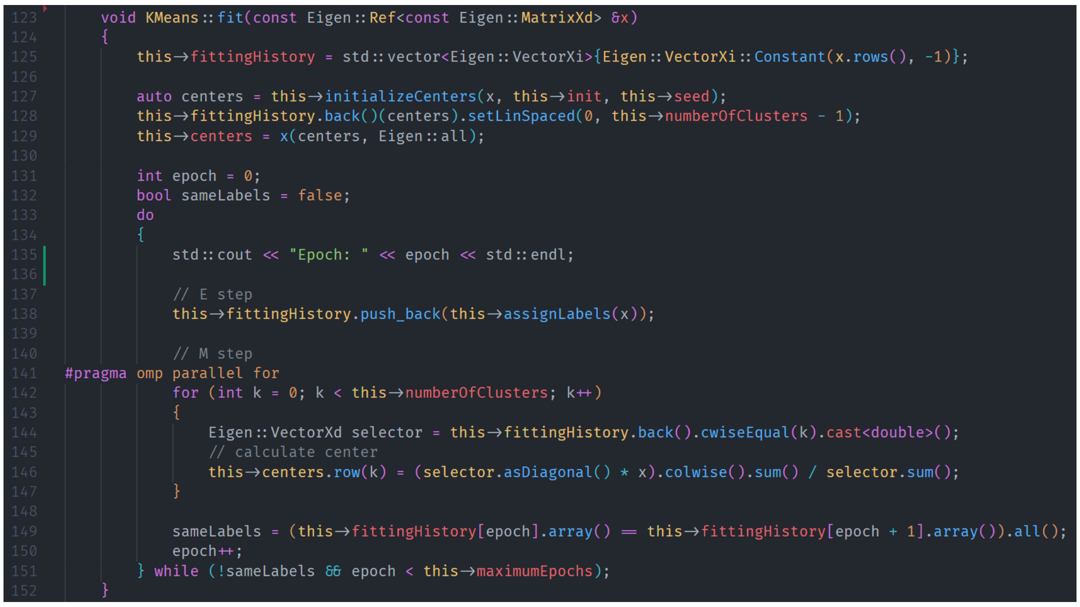


```cpp
    void NormalizedSpectralClustering::fit(const Eigen::Ref<const Eigen::MatrixXd> &x)
    {
        Eigen::DiagonalMatrix<double, Eigen::Dynamic> degreeMatrix = x.rowwise().sum().asDiagonal();

        // L = D - W
        Eigen::MatrixXd laplacianMatrix = -x;
        laplacianMatrix.diagonal() += degreeMatrix.diagonal();

        // solve generalized eigen decomposition
        Eigen::GeneralizedEigenSolver<Eigen::MatrixXd> solver(laplacianMatrix, degreeMatrix, true);
        const Eigen::VectorXcd &eigenValues = solver.eigenvalues();
        const Eigen::MatrixXcd &eigenVectors = solver.eigenvectors();

        std::cout << eigenValues.topRows(5) << std::endl;
        std::cout << eigenVectors.leftCols(5) << std::endl;

        // sort eigenvalues
        std::vector<std::pair<double, Eigen::Index>> eigenPairs(eigenValues.rows());
#pragma omp parallel for
        for (Eigen::Index i = 0; i < eigenValues.rows(); i++)
        {
            eigenPairs[i] = std::make_pair(eigenValues[i].real(), i);
        }
        boost::sort::parallel_stable_sort(eigenPairs.begin(), eigenPairs.end(), this->numberOfThreads);
        // std::partial_sort(eigenPairs.begin(), eigenPairs.begin() + this->numberOfClusters, eigenPairs.end());

        // pick k eigenvectors
        this->eigenMatrix = Eigen::MatrixXd(eigenVectors.rows(), this->numberOfClusters);
#pragma omp parallel for
        for (int i = 0; i < this->numberOfClusters; i++)
        {
            this->eigenMatrix.col(i) = eigenVectors.col(eigenPairs[i].second).real();
        }

        // perform k-means clustering on eigen space
        this->kMeans.fit(this->eigenMatrix);
    }
```

- `kMeans.fit` function: fit the data

> Use the points in eigen space to perform k-means clustering.
>
> Steps
>
> 1. Pick k centers

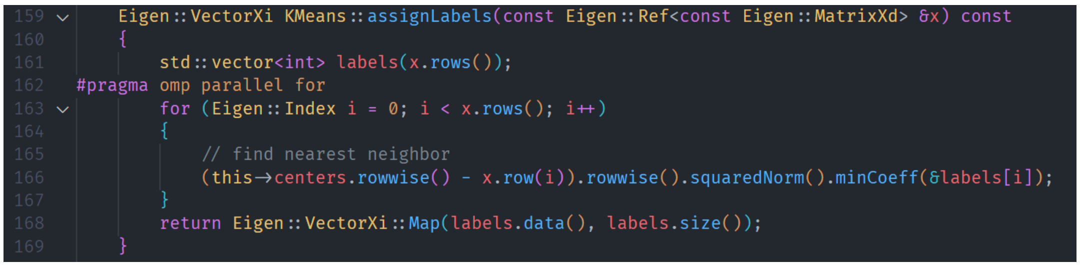
> 2. E step
>   1. Calculate the cost between the data and centers
>   2. Assign the label which has the smallest distance to the data
> 3. M step
>
>   Recalculate the centers by averaging the points which belong to the same cluster.
> 4. Keep repeating 2, 3 step until the labels are not changed



```cpp
void KMeans::fit(const Eigen::Ref<const Eigen::MatrixXd> &x)
{
    this->fittingHistory = std::vector<Eigen::VectorXi>{Eigen::VectorXi::Constant(x.rows(), -1)};

    auto centers = this->initializeCenters(x, this->init, this->seed);
    this->fittingHistory.back()(centers).setLinSpaced(0, this->numberOfClusters - 1);
    this->centers = x(centers, Eigen::all);

    int epoch = 0;
    bool sameLabels = false;
    do
    {
        std::cout << "Epoch: " << epoch << std::endl;

        // E step
        this->fittingHistory.push_back(this->assignLabels(x));

        // M step
#pragma omp parallel for
        for (int k = 0; k < this->numberOfClusters; k++)
        {
            Eigen::VectorXd selector = this->fittingHistory.back().cwiseEqual(k).cast<double>();
            // calculate center
            this->centers.row(k) = (selector.asDiagonal() * x).colwise().sum() / selector.sum();
        }

        sameLabels = (this->fittingHistory[epoch].array() == this->fittingHistory[epoch + 1].array()).all();
        epoch++;
    } while (!sameLabels && epoch < this->maximumEpochs);
}
```

- `assignLabels` function: calculate the cost and assign labels

  > Arguments
  >
  > x: (N, N), the kernel values
  >
  > Steps
  >
  > 1. Calculate the cost (Euclidean distance) between the data and centers
  > 2. Assign the label which has the smallest distance to the data



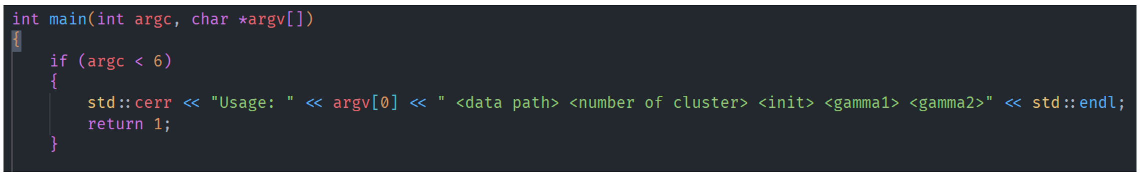
```cpp
Eigen::VectorXi KMeans::assignLabels(const Eigen::Ref<const Eigen::MatrixXd> &x) const
{
    std::vector<int> labels(x.rows());
#pragma omp parallel for
    for (Eigen::Index i = 0; i < x.rows(); i++)
    {
        // find nearest neighbor
        (this->centers.rowwise() - x.row(i)).rowwise().squaredNorm().minCoeff(&labels[i]);
    }
    return Eigen::VectorXi::Map(labels.data(), labels.size());
}
```

Part2

> Use command to control the number of clusters and other parameters.

- **Kernel K-Means**

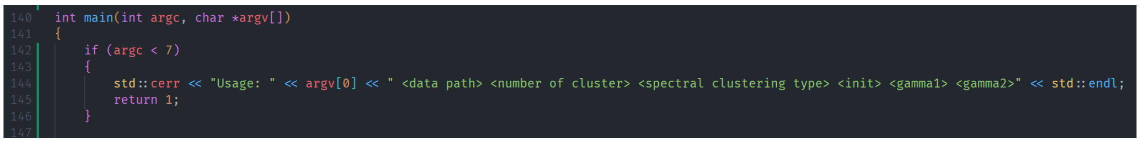
  > init
  >
  > 0 => use random initialization
  >
  > 1 => use k-means++ initialization



```
int main(int argc, char *argv[])
{
    if (argc < 6)
    {
        std::cerr << "Usage: " << argv[0] << " <data path> <number of cluster> <init> <gamma1> <gamma2>" << std::endl;
        return 1;
    }
```

- **Spectral Clustering**

> spectral clustering type
>
> 0 => use spectral clustering algorithm
>
> 1 => use normalized clustering algorithm
>
> init
>
> 0 => use random initialization
>
> 1 => use k-means++ initialization

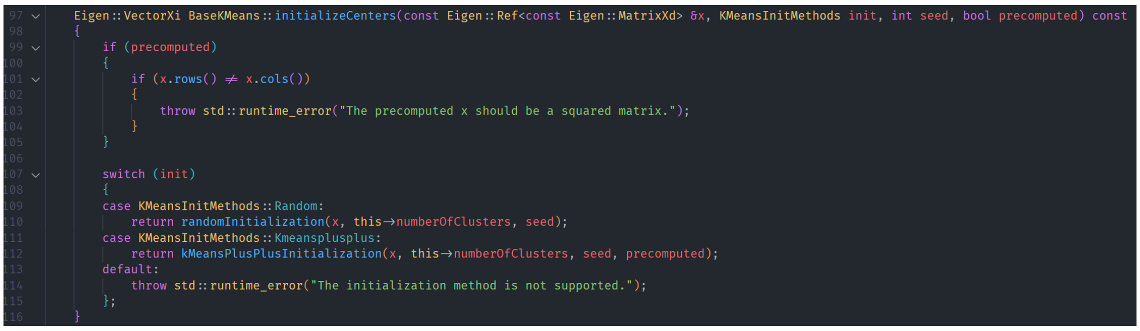


```
int main(int argc, char *argv[])
{
    if (argc < 7)
    {
        std::cerr << "Usage: " << argv[0] << " <data path> <number of cluster> <spectral clustering type> <init> <gamma1> <gamma2>" << std::endl;
        return 1;
    }
```

Part3

- `initializeCenters` function: pick k centers initialized by the selected method

> Arguments
>
> x: (N, N) precomputed distance matrix or (N, features) data
> init: the selected initialization method, random or k-means++
> seed: the random seed
> precomputed: x is the precomputed distance matrix or not.



```
Eigen::VectorXi BaseKMeans::initializeCenters(const Eigen::Ref<const Eigen::MatrixXd> &x, KMeansInitMethods init, int seed, bool precomputed) const
{
    if (precomputed)
    {
        if (x.rows() != x.cols())
        {
            throw std::runtime_error("The precomputed x should be a squared matrix.");
        }
    }

    switch (init)
    {
    case KMeansInitMethods::Random:
        return randomInitialization(x, this->numberOfClusters, seed);
    case KMeansInitMethods::Kmeansplusplus:
        return kMeansPlusPlusInitialization(x, this->numberOfClusters, seed, precomputed);
    default:
        throw std::runtime_error("The initialization method is not supported.");
    };
}
```

- **Random initialization**

> Arguments
>
> x: (N, N) precomputed distance matrix or (N, features) data
> numberOfClusters: k clusters
> seed: the random seed
>
> Steps
>
> 1. generate the sequence of indexes, 0 ~ N-1
> 2. shuffle the sequence
> 3. pick the top k rows as the centers

```cpp
    Eigen::VectorXi randomInitialization(const Eigen::Ref<const Eigen::MatrixXd> &x, int numberOfClusters, int seed)
    {
        auto rng = std::mt19937_64(seed);
        std::vector<int> sequence(x.rows());
        std::iota(sequence.begin(), sequence.end(), 0);
        std::shuffle(sequence.begin(), sequence.end(), rng);

        Eigen::Map<Eigen::VectorXi> tmp = Eigen::VectorXi::Map(sequence.data(), sequence.size());
        return tmp.topRows(numberOfClusters);
    }
```

- **K-Means++ initialization**

> Arguments
>
> x: (N, N) precomputed distance matrix or (N, features) data
>
> numberOfClusters: k clusters
>
> seed: the random seed
>
> Steps
>
> 1. Choose one center uniformly at random among the data points.
> 2. For each data point x not chosen yet, compute $D(x)^2$ (the squared Euclidean distance) or use the precomputed distance matrix, the distance between x and the nearest center that has already been chosen.
> 3. Choose one new data point at random as a new center, using a weighted probability distribution where a point x is chosen with probability proportional to $D(x)^2$. (The farthest point will be chosen.)

```cpp
    Eigen::VectorXi kMeansPlusPlusInitialization(const Eigen::Ref<const Eigen::MatrixXd> &x, int numberOfClusters, int seed, bool precomputed)
    {
        auto rng = std::mt19937_64(seed);
        std::vector<int> candidates;

        // 1. Choose one center uniformly at random among the data points.
        // closed interval [0, rows - 1]
        auto sampler = std::uniform_int_distribution(0, static_cast<int>(x.rows()) - 1);
        candidates.push_back(sampler(rng));
        numberOfClusters--;

        // 2. For each data point x not chosen yet, compute D(x)^2, the distance between x and the nearest center that has already been chosen.
        Eigen::MatrixXd distances(x.rows(), x.rows());
        if (!precomputed)
        {
#pragma omp parallel for
            for (Eigen::Index i = 0; i < x.rows(); i++)
            {
                distances.row(i) = (x.rowwise() - x.row(i)).rowwise().squaredNorm().transpose();
            }
        }
        else
        {
            distances = x;
        }

        auto probabilityDistribution = std::uniform_real_distribution();
        while (numberOfClusters > 0)
        {
            Eigen::Map<Eigen::VectorXi> eigenCandidates = Eigen::VectorXi::Map(candidates.data(), candidates.size());

            // 3. Choose one new data point at random as a new center, using a weighted probability distribution where a point x is chosen with probability proportional to D(x)^2.
            Eigen::VectorXd weights = distances(Eigen::all, eigenCandidates).rowwise().minCoeff();
            weights /= weights.sum();

            auto probability = probabilityDistribution(rng);
            for (int i = 0; i < weights.rows(); i++)
            {
                auto weight = weights[i];
                if (probability < weight)
                {
                    candidates.push_back(i);
                    break;
                }
                probability -= weight;
            }

            numberOfClusters--;
        }
```

Part4

> Visualize the eigen space.

```cpp
void plotEigenSpace(const std::string &path, const Eigen::MatrixXd &eigenMatrix)
{
    matplot::figure();

    const Eigen::VectorXd &vecX = eigenMatrix.col(0);
    const Eigen::VectorXd &vecY = eigenMatrix.col(1);

    std::vector<double> x(vecX.begin(), vecX.end());
    std::vector<double> y(vecY.begin(), vecY.end());
    matplot::scatter(x, y);
    matplot::save(path);
}
```

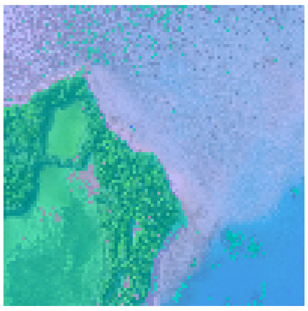
Experiments settings and results & Discussion

Part1

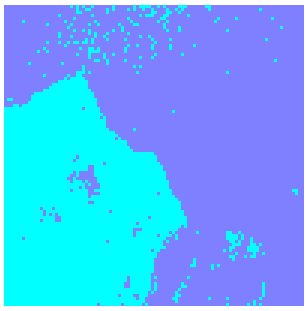
- **Kernel K-Means**

  > Number of clusters: 2
  >
  > Initialization method: random
  >
  > Gamma1: 0.00001
  >
  > Gamma2: 0.00001

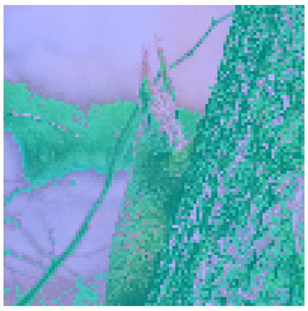
  - image1
    - Video
    - Final

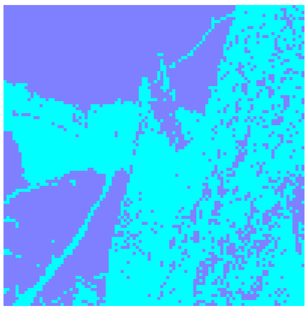
    - Mask

  - image2
    - Video
    - Final

    - Mask



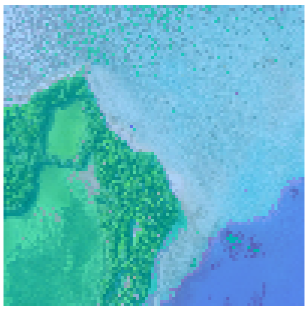
- **Spectral Clustering**

Part2

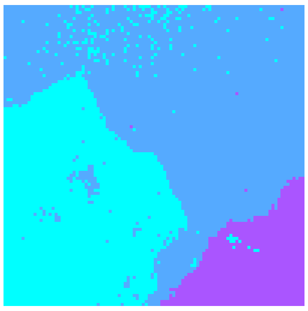
- **Kernel K-Means**

> Initialization method: random
>
> Gamma1: 0.00001
>
> Gamma2: 0.00001

  - K = 3，image1
    - Video
    - Final

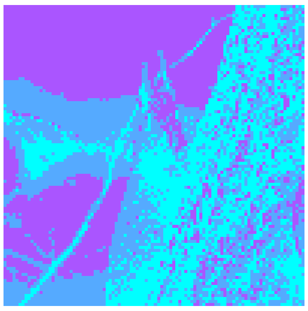


    - Mask

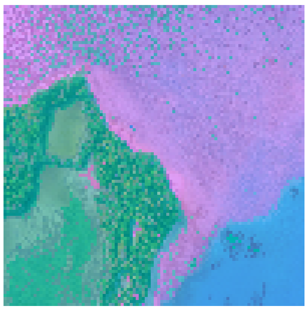


  - K = 3，image2
    - Video
    - Final

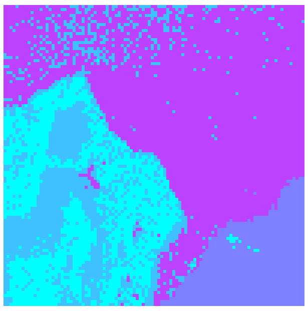
    - Mask



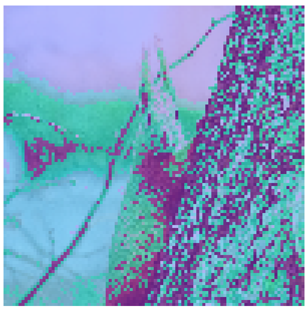
- K = 4 · image1
    - Video
    - Final



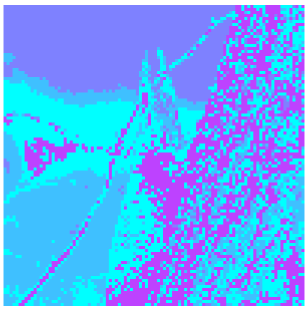
    - Mask



- K = 4 · image2
    - Video
    - Final



    - Mask



- **Spectral Clustering**

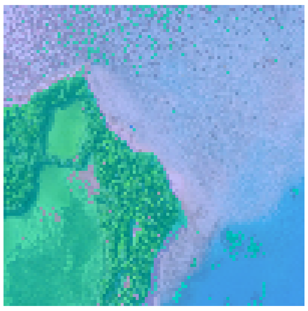
Part3

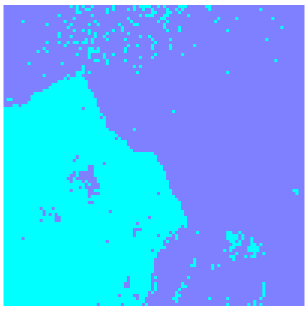
- **Kernel K-Means**

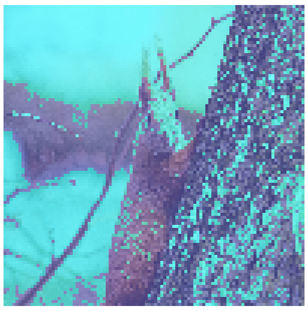
  I think there is no significant difference between random and k-means++.

  > Initialization method: k-means++
  >
  > Gamma1: 0.00001
  >
  > Gamma2: 0.00001

  - K = 2 · image1
    - Video
    - Final

      
    - Mask

      
  - K = 2 · image2
    - Video
    - Final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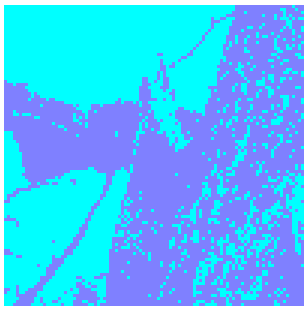
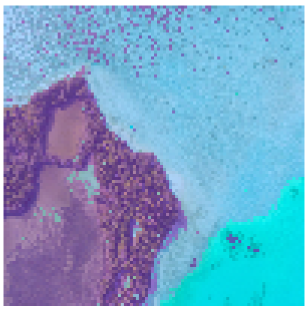
      

- K = 3 · image1
  - Video
  - Final



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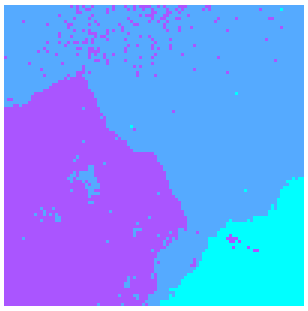
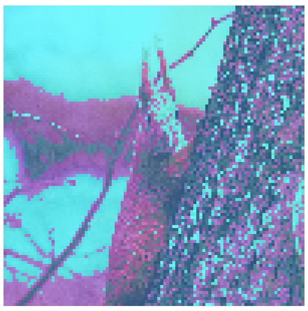
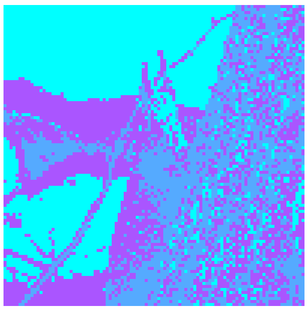


- K = 3 · image2
  - Video
  - Final

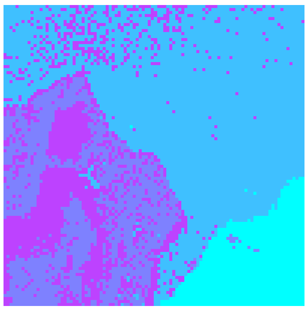


  - Mask



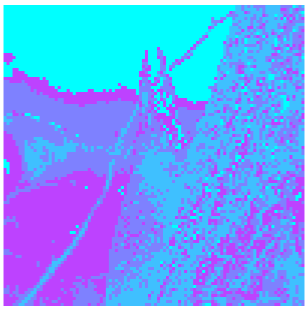
- K = 4 · image1
  - Video
  - Final

- Mask



- K = 4 · image2
  - [Video]
  - Final

  - Mask



- **Spectral Clustering**

Part4

Observations and discussion

- Coming soon...