Pattern Recognition
Lecture 03-2

Gradient Descent & Kernel Trick

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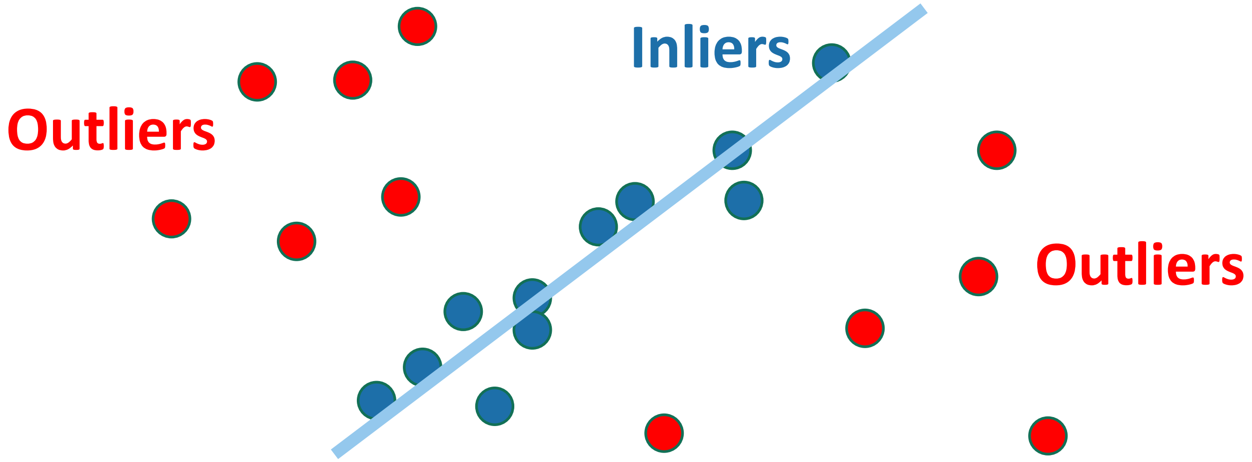
Fall 2022

This Class

- Gradient Descent
- Robust Regression
- Regularization
- **RANSAC**
- **Kernel Trick**

RANSAC

- In computer vision, a widely-used generic framework for robust fitting is random sample consensus (RANSAC)
- This is designed for the scenario where:
  - You have a large number of outliers
  - Majority of points are “Inliners” (Very easy to get low errors on the inliers)



RANSAC

- 1. Sample a small number of training exmples
  - Minimum number needed to fit the model
  - For linear regression with 1 feature, just 2 examples
- 2. Fit the model based on the samples
  - Fit a line to these 2 points
  - With ‘d’ features, you’ll need ‘d+1’ examples
- 3. Test how many points are fit well based on the model
- 4. Repeat until we find a model with the most inliers
- 5. Re-fit the model based on the estimated “inliers”

RANSAC

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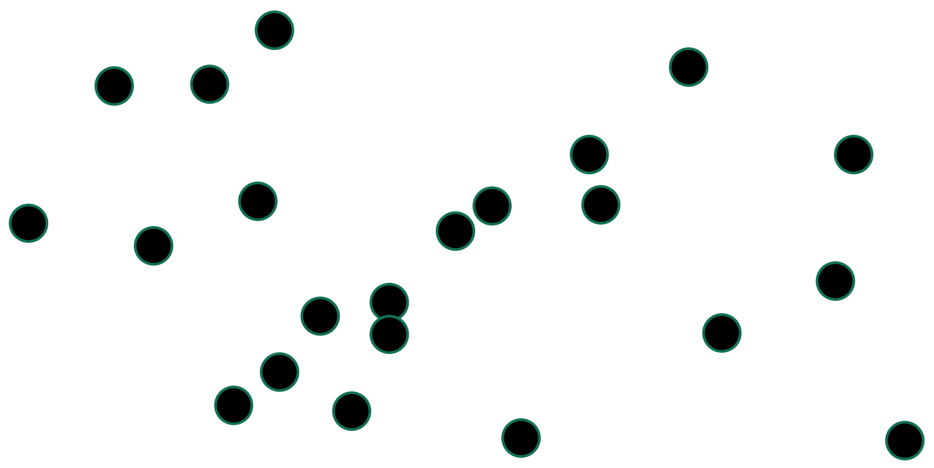

RANSAC

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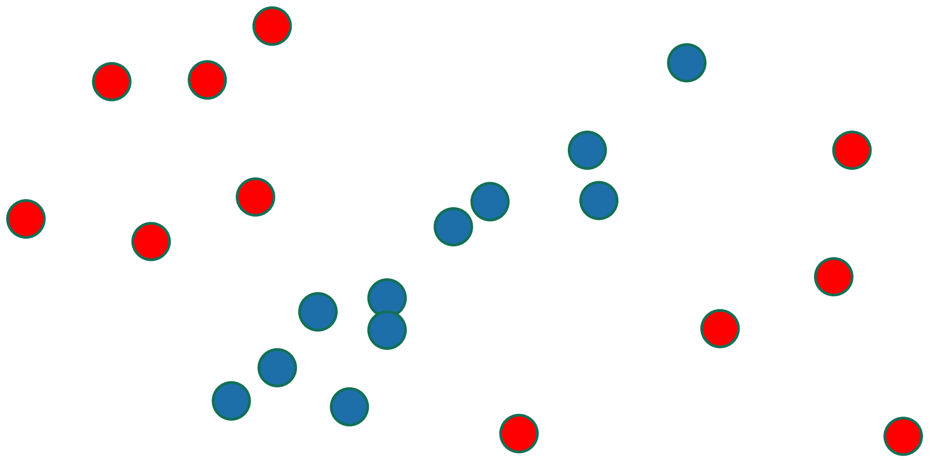
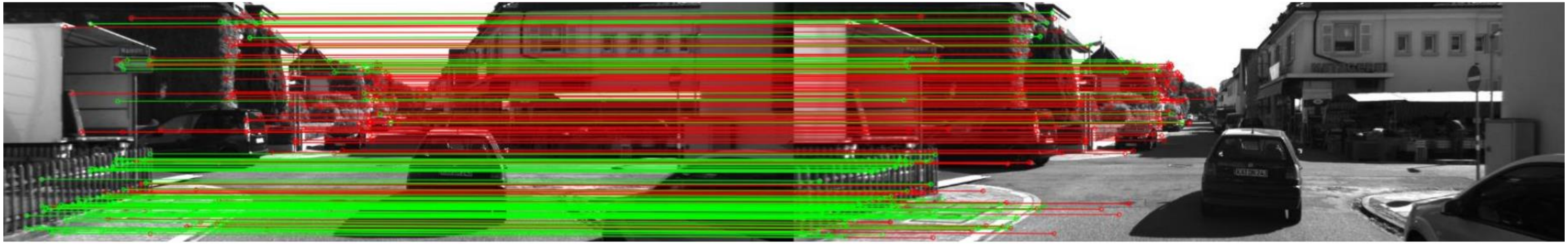
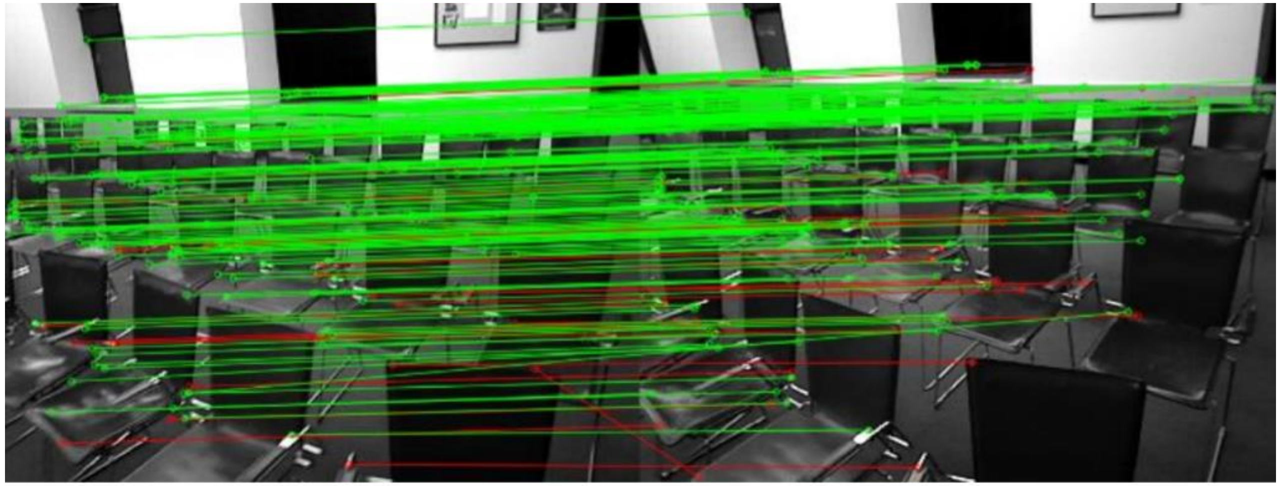


RANSAC - Example

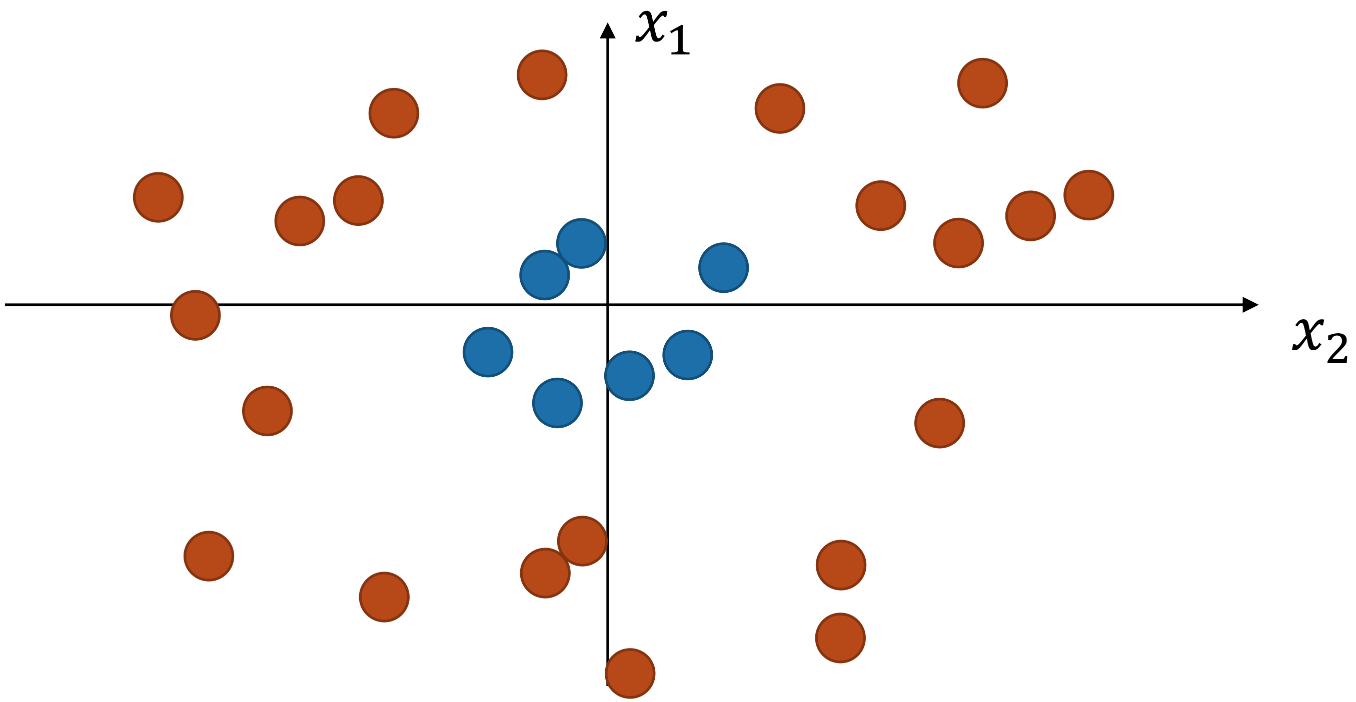
- Structure from motion – Feature matching





Kernel Trick

- Support Vector Machines for Non-separable
  - What should we do for separating the following case?:



Kernel Trick

- Support Vector Machines for Non-separable
  - What should we do for separating the following case:
    - It may be separable under change of basis (ex. $y_i = 2_1 x_{i1}^2 + w_2 \sqrt{2} x_{i1} x_{i2} + w_3 x_{i2}^2$

Multi-dimensional Polynomial Basis

- Recall the fitting polynomials when we only have 1 feature:
  - $\hat{y}_i = w_0 + w_1 x_i + w_2 x_i^2$
- Then, how can we do this when we have a lot of features?
  - It's simple! Consider all of them!
  - $1, x_{i1}, x_{i2}, x_{i3}$
  - $x_{i1}^2, x_{i2}^2, x_{i3}^2$
  - $x_{i1}x_{i2}, x_{i1}x_{i3}, x_{i2}x_{i3}$

Kernel Trick

- If we go to degree p=5, we'll have $O(d^5)$ terms!!
- For large 'd' and 'p', storing a polynomial basis is intractable
  - Z has $k = O(d^p)$ columns, so it does not fit in memory
- Fortunately, we can use all of them with the "kernel trick"

Kernel Trick – L2-regularized Least Squares

- $f(v) = \frac{1}{2}\|\mathbf{Zv} - \mathbf{y}\|^2 + \frac{\lambda}{2}\|\mathbf{v}\|^2$
  - Z : kernel basis
  - v : kernel weights
- Then, $\mathbf{v} = \underbrace{(\mathbf{Z}^T\mathbf{Z} + \lambda\mathbf{I})}_{k \times k}{}^{-1}\mathbf{Z}^T\mathbf{y} = \mathbf{Z}^T\underbrace{(\mathbf{Z}\mathbf{Z}^T + \lambda\mathbf{I})}_{n \times n}{}^{-1}\mathbf{y}$
- This is faster if n<<k:
  - Cost is $O(n^2k + n^3)$ instead of $O(nk^2 + k^3)$
  - But for the polynomial basis, this is still too slow since $k = O(d^p)$

Kernel Trick – L2-regularized Least Squares

- Given test data $\widetilde{\mathbf{X}}$, Predict $\hat{\mathbf{y}}$ by forming $\tilde{\mathbf{Z}}$ and the using:
  - $\hat{\mathbf{y}} = \tilde{\mathbf{Z}}\boldsymbol{v} = \tilde{\mathbf{Z}}\mathbf{Z}^T(\mathbf{Z}\mathbf{Z}^T + \lambda\mathbf{I})^{-1}\mathbf{y} \equiv \widetilde{\mathbf{K}}(\mathbf{K} + \lambda\mathbf{I})^{-1}\mathbf{y}$
  - $\widetilde{\mathbf{K}} \in \mathcal{R}^{t \times n}$
  - $\mathbf{K} + \lambda\mathbf{I} \in \mathcal{R}^{n \times n}$
- Notice that if you have $\mathbf{K}$ and $\widetilde{\mathbf{K}}$ then you do not need $\mathbf{Z}$ and $\tilde{\mathbf{Z}}$
- **Key idea of kernel trick for certain bases:**
  - **We can efficiently compute K and $\widetilde{\mathrm{K}}$**
  - **even though Z and $\tilde{\mathrm{Z}}$ are interactable.**

Kernel Trick – Gram Matrix

- $\mathbf{K} = \mathbf{Z}\mathbf{Z}^T$
  - Contains the dot products between all training examples

- $\widetilde{\mathbf{K}} = \tilde{\mathbf{Z}}\mathbf{Z}^T$
  - Contains the dot products between train and test examples

- Kernel function: $k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{z}_i^T \mathbf{z}_j$

Kernel Trick

- Kernel function: $k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{z}_i^T \mathbf{z}_j$
  - Instead of the acquisition of $\mathbf{z}_i$ and $\mathbf{z}_j$,
  - Directly estimate the Gram matrices from $\mathbf{x}_i$ and $\mathbf{x}_j$

- Linear Kernel: $k(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j = \mathbf{z}_i^T \mathbf{z}_j$
- Polynomial Kernel: $k(\mathbf{x}_i, \mathbf{x}_j) = \left(1 + \mathbf{x}_i^T \mathbf{x}_j\right)^p = \mathbf{z}_i^T \mathbf{z}_j$
- Gaussian-RBF Kernel: $k(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right) = \mathbf{z}_i^T \mathbf{z}_j$

Maximum Likelihood Estimation (MLE)

- $\hat{\mathbf{w}} = \arg\max_{w} p(\mathbf{D}|\mathbf{w})$
  - Example. Coin throwing data = {H,H,T}
    - Likelihood p(HHT | w=0.5) = 0.125
    - Likelihood p(HHT | w=0.0) = 0.0
    - Likelihood p(HHT | w=2/3) = 0.144 (Maximum)
- Minimizing the Negative Log-Likelihood (NLL)
  - $\hat{\mathbf{w}} = \arg\max_{\mathrm{w}} p(\mathbf{D}|\mathbf{w}) = \arg\min_{\mathrm{w}}(-\log p(\mathbf{D}|\mathbf{w}))$
  - Because 'log' is monotonically increasing
  - Then, the likelihood can be represented by addition when i.i.d data are given
    - $\hat{\mathbf{w}} = \arg\min_{w}(-\log \prod_{i=1}^{n} p(\mathbf{D}_i|\mathbf{w})) = \arg\min_{\mathrm{w}}(-\sum_{i=1}^{n} \log p(\mathbf{D}_i|\mathbf{w}))$

Maximum A Priori (MAP)

- $\hat{\mathbf{w}} = \arg\max_{w} p(\mathbf{w}|\mathbf{D})$

- Through Bayes rule and NLL,
  - $p(\mathbf{w}|\mathbf{D}) = \frac{p(\mathbf{D}|\mathbf{w})p(\mathbf{w})}{p(\mathbf{D})} \propto p(\mathbf{D}|\mathbf{w})p(\mathbf{w})$
  - $\hat{\mathbf{w}} = \arg\max_{\mathbf{w}} p(\mathbf{D}|\mathbf{w}) = \arg\min_{\mathbf{w}}(-\log p(\mathbf{D}|\mathbf{w})p(\mathbf{w}))$
  - When i.i.d data are given,
  - $\hat{\mathbf{w}} = \arg\min(-\sum_{i=1}^{n} \log p(\mathbf{D}_i|\mathbf{w}) - \log p(\mathbf{w}))$

MLE vs. MAP

Whose?

- MLE : $\arg\max_{w} p(\mathbf{D}|\mathbf{w})$
  - Classify it based on the hair length, color, shape, etc.
- MAP : $\arg\max_{w} p(\mathbf{w}|\mathbf{D})$
  - Classify it based on the hair length, color, shape, etc. while considering the ratio of cat and dog at the place (Of course, it is very hard to obtain)

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