Convolutional Kernel Networks

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Arthur Gretton's notes

August 6, 2015

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Main ideas: explicitly design feature spaces for ML on images (retrieval, classification) which

- build more complex (hierarchical) feature spaces from simpler ones
- achieve similar local invariance, and fine-to-coarse parts-based features, as convolutional neural nets

The resulting architectures are kernel based (!) and obtain similar performance to CNNs, but much more shallow (2 layers) and with many fewer parameters.

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First: a basic kernel for images

A basic kernel between two images:

- The image is on coordinate space $\Omega_0 = [-1,1]^2$
- A coordinate on the image is $z \in \Omega_0$.
- The feature at z is $\varphi_0(z) \in \mathcal{H}_0$. E.g. vector of RGB values, so $\varphi(z_k) \in \mathbb{R}^3$.

Then a kernel between two images (as described entirely by features φ, φ') is average over kernels at each coordinate pair

$$\mathfrak{K}(\varphi,\varphi') = \sum_{\mathbf{z}\in\Omega} \sum_{\mathbf{z}'\in\Omega} \|\varphi_0(\mathbf{z})\|_{\mathcal{H}_0} \|\varphi'_0(\mathbf{z}')\|_{\mathcal{H}_0} e^{-\frac{1}{\beta^2}\|\mathbf{z}-\mathbf{z}'\|^2} e^{-\frac{1}{\sigma^2}\|\tilde{\varphi}_0(\mathbf{z})-\tilde{\varphi}'_0(\mathbf{z}')\|^2},$$

where

$$ilde{arphi}_{\mathsf{0}}\left(\mathsf{z}
ight) = rac{arphi_{\mathsf{0}}(\mathsf{z})}{\left\|arphi_{\mathsf{0}}(\mathsf{z})
ight\|_{\mathcal{H}_{\mathsf{0}}}}$$

• β is the "local shift invariance" parameter.

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Some useful features:

- $\mathcal{H}_0 = \mathbb{R}^2$ is the 2-D gradient of the image at pixel z. Then $\tilde{\varphi}_0(z)$ is orientation and $\|\varphi_0(z)\|_{\mathcal{H}_0}$ is intensity.
- $\mathcal{H}_0 = \mathbb{R}^{m \times m}$ are the pixel intensities centred at patch z. $\tilde{\varphi}_0(z)$ is contrast-normalized map.

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Next: kernel defined on a Hilbert space input

- The input feature space is defined as φ_{k-1} : $\Omega_{k-1} \to \mathcal{H}_{k-1}$.
 - i.e. the input feature at coordinate $\mathbf{z}_k \in \Omega_{k-1}$ is $\varphi(\mathbf{z}_k)$.
 - From prev. slide: in the case of Ω_0 these are e.g. raw RGB values.
- Define the local patches

$$\{\mathbf{z}_k\} + \mathcal{P}_{k-1} \subset \Omega_{k-1}$$

Define the feature space \mathcal{H}_k at level k, between two patches at level k-1,

$$\begin{split} \mathfrak{K}_{k}(\mathbf{z}_{k},\mathbf{z}_{k}') &= \sum_{\mathbf{z}\in\mathcal{P}_{k}} \sum_{\mathbf{z}'\in\mathcal{P}_{k}} \left\| \varphi_{k-1}(\mathbf{z}_{k}+\mathbf{z}) \right\|_{\mathcal{H}_{k-1}} \left\| \varphi_{k-1}'(\mathbf{z}_{k}'+\mathbf{z}') \right\|_{\mathcal{H}_{k-1}} \\ &\times e^{-\frac{1}{\beta_{k}^{2}} \left\| \mathbf{z}-\mathbf{z}' \right\|^{2}} e^{-\frac{1}{\sigma_{k}^{2}} \left\| \tilde{\varphi}_{k-1}(\mathbf{z}_{k}+\mathbf{z}) - \tilde{\varphi}_{k-1}'(\mathbf{z}_{k}'+\mathbf{z}) \right\|_{\mathcal{H}_{k-1}}^{2}} \\ &= \left\langle \varphi_{k}(\mathbf{z}_{k}), \varphi_{k}'(\mathbf{z}_{k}') \right\rangle_{\mathcal{H}_{k}} \end{split}$$
(1)

- Coordinates \mathbf{z}_k apply to levels Ω_k and Ω_{k-1} .
- Not average kernel on features over whole image just the average on two (local) patches

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Next: kernel defined on a Hilbert space input



Slightly misleading: so far, the number of coordinates z_k is identical at all levels. Also features $\varphi_k(z_k)$ are not known explicitly, infinite dimensional (problem if we want to feed to next layer)

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Approximation of the kernel using sums of features

How to approximate the Gaussian kernel?

The goal is to approximate the kernel by a sum of products of features of the inputs. Start with

$$e^{\frac{-1}{2\sigma^2}\|x-x'\|^2} = \left(\frac{2}{\pi\sigma^2}\right)^{m/2} \int_{w\in\mathbb{R}^m} e^{\frac{-1}{2\sigma}\|x-w\|^2} e^{\frac{-1}{2\sigma}\|x'-w\|^2} dw.$$

In high dimensions, use the approximation

$$\min_{\eta \in \mathbb{R}^{p}_{+}, W \in \mathbb{R}^{m \times p}} \left[\frac{1}{n} \sum_{i=1}^{n} \left(e^{\frac{-1}{2\sigma} \|x_{i} - y_{i}\|^{2}} - \sum_{l=1}^{p} \eta_{l} e^{\frac{-1}{2\sigma} \|x_{i} - w_{l}\|^{2}} e^{\frac{-1}{2\sigma} \|y_{i} - w_{l}\|^{2}} \right)^{2} \right],$$

where (x_i, y_i) are candidate pairs of points on which you want to evaluate the Gaussian.

Approximation of the kernel using sums of features

Relation to neural network nonlinearity: when ||x|| = ||y|| = 1, then ||w|| will be close to 1, and the nonlinear mapping of feature x is

$$u \mapsto e^{(2/\sigma^2)(u-1)}$$
 $u = w^\top x$



 η , W optimized via L-BFGS on 300,000 training points, σ by 0.1 quantile of $(||x_i - y_i||_2)_{i=1}^n$. "Our goal is to demonstrate the preliminary performance of a new type of convolutional network, and we leave as future work any speed improvement."

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Putting it all together

- Inputs from previous layer: represent φ_{k-1}(z) by a vector of length p_{k-1}, written ξ_{k-1}(z).
- Oefine ψ_{k-1}(z_i) to be a patch of these ξ_{k-1} centered at z_i.
 Dimension is ℝ<sup>|P_{k-1}|P_{k-1}. NOT the same feature space as the average over patches in (1).
 </sup>
- **③** Compute a vector of p_k output features at each $z_k \in \Omega_{k-1}$,

$$\zeta_{k}(\mathbf{z}) = \|\psi_{k-1}\|_{2} \left[\sqrt{\eta_{k}} e^{-1/\sigma_{k}^{2}} \|\tilde{\psi}_{k-1}(\mathbf{z}) - \mathbf{w}_{k}\|_{2}^{2} \right]_{l=1}^{p_{k}}$$

 Outputs are pooled with Gaussian weights (after downsampling by a factor of 2),

$$\xi_k(\mathsf{z}) = \sqrt{2/\pi} \sum_{u \in \Omega_{k-1}} e^{-1/\beta_k^2 \|\mathsf{u}-\mathsf{z}\|^2} \zeta_k(\mathsf{z})$$

where the *u* are summed over a grid in Ω_{k-1} .

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Putting it all together



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