Dimension reduction and manifold learning

Deep embeddings, clustering, and label information

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Auto-encoders

Back to coding and decoding

Given a dataset $x_1, \ldots, x_n$, assume the existence of latent variables $z \in \mathbb{R}^d$ of low dimension $d \ll p$ such that $x_i \simeq \mathrm{dec}^*(z_i)$.

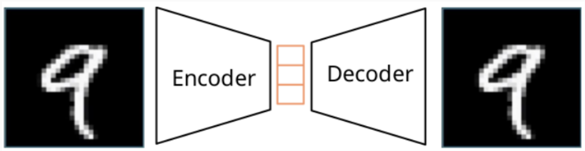
Given a *coder* and $\mathrm{cod} : \mathbb{R}^p \to \mathbb{R}^d$, a *decoder* $\mathrm{dec} : \mathbb{R}^d \to \mathbb{R}^p$

$$\mathbb{R}^p \xrightarrow{\mathrm{cod}} \mathbb{R}^d \xrightarrow{\mathrm{dec}} \mathbb{R}^p.$$

and a loss function $\ell : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$, one can consider the generic reconstruction error

$$\mathcal{E}_{\mathrm{codec}}(\mathrm{cod}, \mathrm{dec}) := \mathbb{E}_x \left[\ell\big(x, \mathrm{dec}(\mathrm{cod}(x))\big) \right].$$

The smallest dimension along the way is called the bottleneck.



PCA considered loss $\ell(x, x') := \|x - x'\|^2$, with linear $\mathrm{cod} = A \in \mathbb{R}^{d \times p}$, $\mathrm{dec} = B \in \mathbb{R}^{p \times d}$

Back to coding and decoding

Given a *coder* architecture $\mathrm{cod}_\theta : \mathbb{R}^p \to \mathbb{R}^d$ and a *decoder* architecture $\mathrm{dec}_\phi : \mathbb{R}^d \to \mathbb{R}^p$, define the population reconstruction risk

$$\mathcal{E}(\theta, \phi) := \mathbb{E}\big[\ell\big(x,\ \mathrm{dec}_\phi(\mathrm{cod}_\theta(x))\big)\big] \, .$$

for $\theta \in \Theta$ and $\phi \in \Xi$.

Training problem (ERM). Given samples $x_1, \ldots, x_n$,

$$(\hat{\theta}, \hat{\phi}) \in \operatorname*{arg\,min}_{\theta,\phi} \ \frac{1}{n} \sum_{i=1}^{n} \ell\big(x_i, \mathrm{dec}_\phi(\mathrm{cod}_\theta(x_i))\big).$$

Squared loss and basic calculus

Write the reconstruction map

$$r_{\theta,\phi}(x) := \operatorname{dec}_\phi(\operatorname{cod}_\theta(x)) \in \mathbb{R}^p.$$

If $\ell(x, \hat{x}) = \|x - \hat{x}\|^2$, then

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For differentiable $\mathrm{cod}_\theta, \mathrm{dec}_\phi$ and any perturbation δr,

$$\delta\mathcal{E} = 2\,\mathbb{E}\big[\langle r(x) - x,\ \delta r(x)\rangle\big].$$

Hence stationarity is governed by the orthogonality condition

$$\mathbb{E}\big[(x - r(x))\,\delta r(x)^\top\big] = 0 \quad \text{for all admissible perturbations } \delta r.$$

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$\hookrightarrow$ This becomes explicit for linear auto-encoders.

Linear auto-encoder, aka PCA

Assuming centered data $\mathbb{E}[x] = 0$, consider a linear coder/decoder:

$$\mathrm{cod}(x) = Ax, \quad A \in \mathbb{R}^{d\times p}, \qquad \mathrm{dec}(z) = Bz, \quad B \in \mathbb{R}^{p\times d},$$

so that $r(x) = BAx$.

The population risk becomes

$$\mathcal{E}(A,B) = \mathbb{E}\big[\|x - BAx\|^2\big] = \mathrm{Tr}(\Sigma) - 2\,\mathrm{Tr}(BA\Sigma) + \mathrm{Tr}(BA\Sigma A^\top B^\top),$$

where $\Sigma := \mathbb{E}[xx^\top]$.

For fixed A, the objective is quadratic in B. Differentiating w.r.t. B gives the normal equation

$$-2A\Sigma + 2BA\Sigma A^\top = 0 \quad \Longrightarrow \quad B^\star(A) = \Sigma A^\top (A\Sigma A^\top)^{-1} \quad \text{(if } A\Sigma A^\top \text{ invertible).}$$

Plugging back yields a function of the subspace $\mathrm{Im}(A^\top)$ only:

$$\begin{aligned}\mathcal{E}(A, B^\star(A)) &= \mathrm{Tr}(\Sigma) - \mathrm{Tr}\big(\Sigma A^\top (A\Sigma A^\top)^{-1} A\Sigma\big)\\ &= \mathrm{Tr}(\Sigma) - \mathrm{Tr}\big(\mathrm{proj}_{\Sigma^{1/2}\mathrm{Im}(A^\top)}\Sigma\big).\end{aligned}$$

Non-identifiability and normalization constraints

Even at a global optimum, (A, B) is not unique.

If $Q \in \mathbb{R}^{d\times d}$ is invertible, then

$$Ax \mapsto QAx, \qquad Bz \mapsto BQ^{-1}z$$

keeps the reconstruction BAx unchanged.

Common normalizations (to fix a gauge).

- Tied weights: $B = A^\top$ (which we used for PCA earlier in the course).
- Whitening of codes: $\mathbb{E}[zz^\top] = A\Sigma A^\top = I_d$ (or empirically $Z^\top Z = I_d$).
- Orthogonality: $AA^\top = I_d$ (restricts A to an orthogonal projection).

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$\hookrightarrow$ For nonlinear AEs, such constraints become implicit via regularization terms / architecture choice).

The simplest non-linear auto-encoder (historical perspective)

A first non-linear extension of PCA is an undercomplete (i.e. $d \ll p$) 1-hidden-layer network (**bourlard1988autoassociation**)

$$x \in \mathbb{R}^p \xrightarrow{\mathrm{cod}_\theta} z = \sigma(Wx + b) \in \mathbb{R}^d \xrightarrow{\mathrm{dec}_\phi} \hat{x} = \tau(Vz + c) \in \mathbb{R}^p.$$

with activations σ, τ (e.g. sigmoid / $\tanh$ / ReLU) and parameters $\theta = (W, b)$, $\phi = (V, c)$.

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Key point. Unlike the linear case, even with $d \ll p$, nonlinearity can adapt the reconstruction map $r(x) = \mathrm{dec}_\phi(\mathrm{cod}_\theta(x))$ to *curved* low-dimensional structure.

Architectures and losses

Architectures. (Goodfellow, Bengio, and Courville 2016)

- MultiLayer Perceptron: compositions of affine maps and pointwise nonlinearities.
- Convolutional: replace affine maps by convolutions (translation equivariance).
- Residual / U-Net: skip connections to improve optimization and preserve fine-scale details. (He et al. 2016; Ronneberger, Fischer, and Brox 2015)

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Losses.

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- Bernoulli model (binary data): $\ell(x, \hat{x}) = -\sum_{j=1}^{p} \left(x_j \log \hat{x}_j + (1 - x_j) \log(1 - \hat{x}_j)\right)$ with $x, \hat{x} \in (0,1)^p$ (e.g. $\tau = \mathrm{sigmoid}$).
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Optimization.

- Training uses gradient methods (SGD/Adam): backprop computes $\nabla_\theta \ell(x_i, r_{\theta,\phi}(x_i))$ and $\nabla_\phi \ell(x_i, r_{\theta,\phi}(x_i))$ by the chain rule, where $r_{\theta,\phi}(x) := \mathrm{dec}_\phi(\mathrm{cod}_\theta(x))$.

Why regularization is not optional (nonlinear case)

If $\mathrm{cod}, \mathrm{dec}$ are too expressive, the trivial solution $r(x) \approx x$ on the training set may occur: memorization (think of a Hilbert space-filling curve).

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A standard approach is to penalize complexity and/or enforce structure:

$$\min_{\theta,\phi} \ \frac{1}{n}\sum_{i=1}^{n} \ell\big(x_i, r_{\theta,\phi}(x_i)\big) \ + \ \lambda\, \mathrm{pen}(\theta,\phi).$$

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Typical choices of pen: (Goodfellow, Bengio, and Courville 2016, Chapter 14)

- Weight decay: $\mathrm{pen} = \|\theta\|_2^2 + \|\phi\|_2^2$
- Sparse codes: add $\lambda_s \, \mathbb{E}[\|z(x)\|_1]$ or a KL penalty toward a target sparsity if $z \in (0,1)^d$
- Contractive penalty (stability of the encoder): $\lambda_c \, \mathbb{E}[\|\nabla_x z(x)\|_{\mathrm{F}}^2]$ (Rifai et al. 2011)

Deep auto-encoders and layerwise training

Deep AEs use multiple layers:

$$\mathrm{cod}_\theta = f_L \circ \cdots \circ f_1, \qquad \mathrm{dec}_\phi = g_1 \circ \cdots \circ g_L,$$

with $f_\ell(x) = \sigma(W_\ell x + b_\ell)$, etc.

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A historically important practical difficulty: optimization (vanishing gradients in early deep nets). A classical workaround was layerwise pretraining: (Bengio et al. 2007; Hinton and Salakhutdinov 2006)

- Train a shallow AE on x to produce $z^{(1)}$.
- Train a second AE on $z^{(1)}$ to produce $z^{(2)}$.
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Insight. Pretraining provides an initialization that already approximately preserves information layer by layer. Then, fine-tuning optimizes the end-to-end reconstruction.

More recent AE methods

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Three common directions.

- Geometric regularization: combine reconstruction with Jacobian penalties / Lipschitz control to obtain stable embeddings.
- Latent prior matching: encourage the empirical latent code distribution to match a target prior while still reconstructing. (Gretton et al. 2012; Makhzani et al. 2016)
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These modifications can be written in a unified way:

$$\min_{\theta,\phi} \; \mathbb{E}[\ell_{\text{rec}}(x, r(x))] \; + \; \lambda_1 \, \mathcal{R}_{\text{geom}}(\theta) \; + \; \lambda_2 \, \mathcal{R}_{\text{latent}}(z_\theta(x)) \; + \; \lambda_3 \, \mathcal{R}_{\text{sup}}(z_\theta(x), y).$$

Implicit regularization via noise injection

To regularize implicitly, a Denoising Auto-Encoder (Vincent et al. 2008) replaces the clean input x by a *intentionally* corrupted one $\tilde{x} = x + \varepsilon$ and simply trains

$$\mathcal{E}_\sigma(r) = \mathbb{E}\big[\|x - r(x+\varepsilon)\|^2\big], \qquad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_p).$$

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Heuristic: Assuming r is C^2 and expanding around x,

$$\|x - r(x+\varepsilon)\|^2 = \|x - r(x)\|^2 - 2\langle x - r(x), \nabla r(x)\varepsilon\rangle + \|\nabla r(x)\varepsilon\|^2 + O(\|\varepsilon\|^3).$$

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Taking expectation over ε conditionally on x gives

$$\mathbb{E}_\varepsilon[\langle x - r(x), \nabla r(x)\varepsilon\rangle \mid x] = 0, \qquad \mathbb{E}_\varepsilon[\|\nabla r(x)\varepsilon\|^2 \mid x] = \sigma^2 \|\nabla r(x)\|_{\mathrm{F}}^2.$$

Therefore, for small σ,

$$\mathcal{E}_\sigma(r) = \mathbb{E}\big[\|x - r(x)\|^2\big] + \sigma^2\, \mathbb{E}\big[\|\nabla r(x)\|_{\mathrm{F}}^2\big] + O(\sigma^3),$$

so denoising acts like a contractive regularization on the reconstruction map. (Bishop 1995)

$\hookrightarrow$ Next: the exact optimality statement for DAEs (posterior mean).

Denoising auto-encoders: objective and first-order optimality

An optimal denoising auto-encoder (DAE) learns to reconstruct x from a corrupted version $\tilde{x}$

$$\tilde{x} := x + \varepsilon, \qquad \varepsilon \sim \mathcal{N}(0, \sigma^2 I_p) \text{ independent of } x,$$

by minimizing $\mathcal{E}_\sigma(r) := \mathbb{E}\big[\|x - r(\tilde{x})\|^2\big]$ over $r : \mathbb{R}^p \to \mathbb{R}^p$ measurable.

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Conditioning on $\tilde{x}$:

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For each $\tilde{x}$, the inner expectation is minimized by $r^\star_\sigma(\tilde{x}) := \mathbb{E}[x \mid \tilde{x}]$.

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Thus, an ideal DAE estimates the posterior mean $\mathbb{E}[x \mid \tilde{x}]$ ($\sim$ regression problem).

DAE & score-like vector field

Theorem ((Alain and Bengio 2014), informal)

Let p be the density of x, and $p_\sigma := p * \mathcal{N}(0, \sigma^2 I)$ the density of $\tilde{x} = x + \varepsilon$. For squared loss, the optimal denoiser satisfies

$$r^\star_\sigma(\tilde{x}) - \tilde{x} = \sigma^2 \nabla \log p_\sigma(\tilde{x}).$$

In particular, if p is smooth and σ is small,

$$r^\star_\sigma(x) \approx x + \sigma^2 \nabla \log p(x).$$

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Idea of proof. Since $r_\sigma^\star(\tilde{x}) = \mathbb{E}[x \mid \tilde{x}]$, it is enough to relate the posterior mean shift to $\nabla \log p_\sigma$. Write

$$p_\sigma(\tilde{x}) = \int p(x)\, \mathcal{N}(\tilde{x}; x, \sigma^2 I)\, dx, \qquad \nabla_{\tilde{x}} \mathcal{N}(\tilde{x}; x, \sigma^2 I) = -\frac{\tilde{x} - x}{\sigma^2} \mathcal{N}(\tilde{x}; x, \sigma^2 I).$$

Differentiate under the integral:

$$\nabla \log p_\sigma(\tilde{x}) = \frac{\nabla p_\sigma(\tilde{x})}{p_\sigma(\tilde{x})} = -\frac{1}{\sigma^2} \frac{\int (\tilde{x} - x)\, p(x) \mathcal{N}(\tilde{x}; x, \sigma^2 I)\, dx}{\int p(x) \mathcal{N}(\tilde{x}; x, \sigma^2 I)\, dx} = \frac{1}{\sigma^2}\, \mathbb{E}[x - \tilde{x} \mid \tilde{x}].$$

Contractive regularization: a geometric reading

A contractive AE penalizes sensitivity of the code to input perturbations explicitly.

Let $z(x) := \mathrm{cod}_\theta(x) \in \mathbb{R}^d$, and write $J_z(x) := \nabla_x z(x) \in \mathbb{R}^{d\times p}$.

A common objective is

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Qualitative effect. If x lies near a d-dimensional manifold $M \subset \mathbb{R}^p$, the penalty $\|J_z(x)\|_{\mathrm{F}}^2$ encourages z to be (locally) insensitive to directions orthogonal to M: small changes in x that do not stay on M should not change the representation.

$\hookrightarrow$ Connecting with manifold learning.

Supervised regularization: multi-objective learning

Given labels y (classification or regression), add a supervised head $h_\psi : \mathbb{R}^d \to \mathcal{Y}$ and optimize

$$\min_{\theta,\phi,\psi} \mathbb{E}\big[\ell_{\text{rec}}(x, r(x))\big] + \lambda\,\mathbb{E}\big[\ell_{\text{sup}}(h_\psi(z(x)), y)\big].$$

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Limiting regimes.

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$\hookrightarrow$ For representation learning, λ is chosen by validating downstream performance of z.

Practice: diagnostics and failure modes

Key hyperparameters:

- bottleneck d,
- architecture depth/width,
- noise level σ (DAE),
- Jacobian weight λ (CAE),
- supervised weight λ.

Diagnostics:

- Reconstruction: $\frac{1}{n}\sum_i \ell(x_i, \hat{x}_i)$ and its generalization gap.
- Latent covariance: $\widehat{\Sigma}_z := \frac{1}{n}\sum_i (z_i - \bar{z})(z_i - \bar{z})^\top$ (collapse $\Leftrightarrow$ low rank).
- Local stability: $\|J_z(x_i)\|_{\mathrm{F}}$ (contractive effect), or $\|r(x_i + \delta) - r(x_i)\|$ for small δ.

Typical failure modes:

- overcomplete memorization (too large d / too expressive decoder),
- representation collapse (too strong regularization),
- label leakage (too large supervised weight).

Variational auto-encoders

From reconstructing points to modeling distributions

A classical auto-encoder learns a deterministic reconstruction map

$$x \in \mathbb{R}^p \xrightarrow{\mathrm{cod}_\phi} z \in \mathbb{R}^d \xrightarrow{\mathrm{dec}_\theta} \hat{x} \in \mathbb{R}^p, \qquad \hat{x} := r_{\theta,\phi}(x) = \mathrm{dec}_\theta(\mathrm{cod}_\phi(x)),$$

typically by minimizing a reconstruction loss $\mathbb{E}[\ell(x, \hat{x})]$.

Question. Beyond reconstruction, can we *model the population* that generated the data, and *sample new observations*?

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typically by minimizing a reconstruction loss $\mathbb{E}[\ell(x, \hat{x})]$.

Question. Beyond reconstruction, can we *model the population* that generated the data, and *sample new observations*?

$\hookrightarrow$ A Variational Auto-Encoder answers this by making the decoder a *likelihood model*.

Jointly introduced by (Kingma and Welling 2014; Rezende, Mohamed, and Wierstra 2014)

VAE: latent variable model and decoder as likelihood

Assume a latent variable model

$$Z \sim p(z) \quad \text{(prior on latent space)}, \qquad X \mid (Z = z) \sim p_\theta(x \mid z) \quad \text{(decoder / likelihood)}.$$

The joint density is

$$p_\theta(x, z) = p_\theta(x \mid z)\, p(z), \qquad \text{hence} \qquad p_\theta(x) = \int_{\mathbb{R}^d} p_\theta(x \mid z)\, p(z)\, \mathrm{d}z.$$

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Typical choices.

- $p(z) = \mathcal{N}(0, I_d)$,
- $p_\theta(x \mid z) = \mathcal{N}(\mu_\theta(z), \sigma_x^2 I_p)$ (Gaussian decoder),
- or $p_\theta(x \mid z) = \prod_{j=1}^{p} \mathrm{Bernoulli}(\pi_{\theta,j}(z))$ (binary data).

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Objective. Fit θ by maximum likelihood: $\max_\theta \sum_{i=1}^{n} \log p_\theta(x_i)$,
Problem. $\log p_\theta(x)$ involves an intractable integral in general.

Variational inference: Jensen lower bound

Introduce an auxiliary density $q(z \mid x)\mathrm{d}z$. Then

$$\begin{aligned}
\log p_\theta(x) &= \log \int p_\theta(x, z)\, \mathrm{d}z \\
&= \log \int q(z \mid x)\, \frac{p_\theta(x, z)}{q(z \mid x)}\, \mathrm{d}z \\
&= \log \mathbb{E}_{z \sim q(\cdot \mid x)} \left[\frac{p_\theta(x, z)}{q(z \mid x)} \right] \\
&\geq \mathbb{E}_{z \sim q(\cdot \mid x)} \left[\log \left(\frac{p_\theta(x, z)}{q(z \mid x)} \right) \right] \\
&= \mathbb{E}_{z \sim q(\cdot \mid x)} [\log p_\theta(x, z) - \log q(z \mid x)]\,,
\end{aligned}$$

by Jensen's inequality.

Definition (Evidence Lower BOund – ELBO (Kingma and Welling 2014))

For any $q(z \mid x)\mathrm{d}z$, define

$$\mathrm{ELBO}_\theta(q; x) := \mathbb{E}_{z \sim q(\cdot \mid x)}\left[\log p_\theta(x, z) - \log q(z \mid x)\right].$$

We have $\mathrm{ELBO}_\theta(q; x) \leq \log p_\theta(x)$. (Evidence is just Bayesian name for the marginal likelihood $p_\theta(x)$)

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Object	Name
$p(z)$	Prior
$p_\theta(x \mid z)$	Likelihood / Decoder distribution
$p_\theta(x, z)$	Joint model
$p_\theta(x)$	Marginal likelihood / Evidence
$p_\theta(z \mid x)$	True posterior
$q(z \mid x)$	Variational posterior / Approximate posterior
$q_\phi(z \mid x)$	Encoder distribution
$\mathrm{ELBO}_\theta(q; x)$	Evidence Lower Bound (ELBO)

ELBO decomposition and the two terms

Using $p_\theta(x, z) = p_\theta(x \mid z)p(z)$,

$$\mathrm{ELBO}_\theta(q; x) = \mathbb{E}_{q(z|x)}[\log p_\theta(x \mid z)] - \mathrm{KL}\big(q(z \mid x) \,\|\, p(z)\big).$$

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Moreover, the gap to the log-likelihood is an explicit KL divergence:

$$\log p_\theta(x) - \mathrm{ELBO}_\theta(q;x) = \mathrm{KL}\big(q(z \mid x) \,\|\, p_\theta(z \mid x)\big) \;\geq\; 0,$$

so maximizing the ELBO pushes $q(z \mid x)$ towards the true posterior $p_\theta(z \mid x)$.

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Interpretation.

- $\mathbb{E}_q[\log p_\theta(x \mid z)]$ = reconstruction / data-fit term,
- $\mathrm{KL}(q(z \mid x) \| p(z))$ = regularization enforcing a structured latent space (matching the prior).

VAE training objective (amortized variational family)

In practice, choose a parametric family $q_\phi(z \mid x)$ (the encoder), and optimize

$$\max_{\theta,\phi} \frac{1}{n}\sum_{i=1}^{n} \mathrm{ELBO}_\theta(\phi; x_i), \qquad \mathrm{ELBO}_\theta(\phi; x) = \mathbb{E}_{z\sim q_\phi(\cdot\mid x)}[\log p_\theta(x \mid z)] - \mathrm{KL}\big(q_\phi(z \mid x) \,\|\, p(z)\big).$$

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Gaussian encoder (standard choice).

$$q_\phi(z \mid x) = \mathcal{N}\big(\mu_\phi(x), \mathrm{diag}(\sigma_\phi(x)^2)\big).$$

The KL term to $p(z) = \mathcal{N}(0, I_d)$ is available in closed-form:

$$\mathrm{KL}\big(q_\phi(z \mid x) \,\|\, \mathcal{N}(0, I)\big) = \frac{1}{2}\sum_{k=1}^{d} \big(\mu_{\phi,k}(x)^2 + \sigma_{\phi,k}(x)^2 - \log \sigma_{\phi,k}(x)^2 - 1\big)\,.$$

Reparameterization trick (enabling backprop through sampling)

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where $\odot$ is the coordinatewise product.

Then, for a Monte-Carlo draw ε,

$$\mathbb{E}_{z \sim q_\phi(\cdot \mid x)}[\log p_\theta(x \mid z)] = \mathbb{E}_{\varepsilon \sim \mathcal{N}(0,I)} \left[\log p_\theta(x \mid \mu_\phi(x) + \sigma_\phi(x) \odot \varepsilon) \right],$$

which is differentiable w.r.t. (θ, ϕ) and amenable to SGD.

How VAEs relate to classical AEs

Assume a Gaussian decoder

$$p_\theta(x \mid z) = \mathcal{N}(\mu_\theta(z), \sigma_x^2 I_p).$$

Then (up to an additive constant)

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Thus, maximizing the ELBO is equivalent to minimizing (up to constants)

$$\underbrace{\mathbb{E}_{z\sim q_\phi(\cdot|x)}\left[\|x - \mu_\theta(z)\|^2\right]}_{\text{reconstruction}} + \underbrace{2\sigma_x^2\,\mathrm{KL}\big(q_\phi(z \mid x)\,\|\,p(z)\big)}_{\text{latent regularization}}.$$

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Heuristic. If $q_\phi(z \mid x)$ becomes highly concentrated, the first term resembles a classical AE loss, but the KL forces the encoder's output distribution to stay close to the prior.

Generation: what a VAE gives that an AE does not

Once trained, a VAE defines a full generative model:

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Take-home.
$\hookrightarrow$ A classical AE learns *a reconstruction map*.
$\hookrightarrow$ A VAE learns *a probability model* of the population, enabling principled sampling.

VAE vs DAE: two drastically different ways to use noise

VAE noise (latent). Randomness is introduced in $z \sim q_\phi(z \mid x)$ to optimize a variational bound, and the KL term structures the latent space.

$\hookrightarrow$ *models* $p_\theta(x)$ via latent-variable likelihoods and ELBOs.

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$\hookrightarrow$ *models* $p_\theta(x)$ via latent-variable likelihoods and ELBOs.

DAE noise (input). Randomness is introduced at the input $\tilde{x} = x + \varepsilon$, and the network is trained to *denoise*:

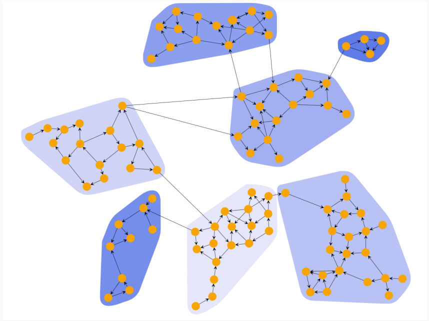
$$\min_r \ \mathbb{E}\left[\|x - r(\tilde{x})\|^2\right].$$

$\hookrightarrow$ *learns* a reconstruction/denoising operator.

Dimension reduction & clustering

Graph clustering

Given an unlabeled undirected weighted graph $\mathcal{G} = (V, W)$ with $|V| = n$ nodes and weight matrix $W \in \mathbb{R}^{n \times n}$, we would like to *decompose* it “as best as possible” into K clusters.



Here, W is a similarity matrix, i.e. $w_{i,j}$ is $\begin{cases} \text{large} & \text{if } i \text{ and } j \text{ are close / well-connected,} \\ \text{small} & \text{otherwise.} \end{cases}$

$\hookrightarrow$ For instance, one may take a binary adjacency matrix $w_{i,j} = \mathbf{1}_{i \sim j}$.

Graph cut

Idea: find clusters that are internally dense and separated by few cross-edges.

Given a candidate partition $V_1, \ldots, V_K$ of V, its cut value is

$$\mathrm{Cut}_W(V^{(1)}, \ldots, V^{(K)}) := \frac{1}{2} \sum_{k=1}^{K} \mathrm{Cut}_W(V^{(k)}), \quad \text{where } \mathrm{Cut}_W(V^{(k)}) := \sum_{\substack{i \in V^{(k)} \\ j \in (V^{(k)})^c}} w_{i,j}.$$

The graph cut counts each cross-edge once.

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Unfortunately, a partition minimizing $\mathrm{Cut}_W(V^{(1)}, \ldots, V^{(K)})$ typically is very unbalanced:

$\hookrightarrow$ $(K-1)$ singletons $V^{(k)} = \{v_{i_k}\}$ of lowest degree $d_{i_k} := \sum_{j \in V} w_{i_k,j}$,

$\hookrightarrow$ $V^{(K)}$ being the remaining $n-K$ nodes.

Normalized graph cut

To *penalize* uneven clusters, consider the normalized cut

$$\mathrm{NCut}_W(V^{(1)}, \dots, V^{(K)}) := \frac{1}{2} \sum_{k=1}^{K} \frac{\mathrm{Cut}_W(V^{(k)})}{\mathrm{Vol}(V^{(k)})}, \quad \text{where } \mathrm{Vol}(V^{(k)}) := \sum_{i \in V^{(k)}} d_i.$$

This loss leads to the minimization problem

$$\operatorname*{arg\,min}_{(V^{(1)}, \dots, V^{(K)})} \mathrm{NCut}_W(V^{(1)}, \dots, V^{(K)}).$$

This problem called `NCUT` is unfortunately NP-complete (Shi and Malik 2000).

However, we can try and find a computationally simpler convex relaxation of it.

Convexifying the normalized graph cut

To convexify the problem, we shall replace each partition element $V^{(k)}$ by its (normalized) indicator function.

Namely, define the normalized cluster indicator $v^{(k)} \in \mathbb{R}^n$ and degree matrix $D \in \mathbb{R}^{n\times n}$ by

$$v_i^{(k)} := \begin{cases} 1/\sqrt{\mathrm{Vol}(V^{(k)})} & \text{if } i \in V^{(k)}, \\ 0 & \text{otherwise.} \end{cases}, \quad \text{and} \quad D := \mathrm{diag}(d_1, \ldots, d_n) \in \mathbb{R}^{n\times n}$$

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– In $\mathbb{R}^n$, for all $k \neq k' \leq K$, we have:

  – $\langle v^{(k)}, Dv^{(k)} \rangle = 1$,
  – $\langle v^{(k)}, Dv^{(k')} \rangle = 0$, since $V^{(k)} \cap V^{(k')} = \emptyset$.

– The normalized cut can be rewritten as

$$\mathrm{NCut}_W(v^{(1)}, \dots, v^{(K)}) = \frac{1}{2} \sum_{k=1}^{K} \sum_{\substack{i \in V^{(k)} \\ j \in (V^{(k)})^c}} \frac{w_{i,j}}{\mathrm{Vol}(V^{(k)})} = \frac{1}{2} \sum_{k=1}^{K} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{i,j} (v_i^{(k)} - v_j^{(k)})^2.$$

Graph Laplacian

On the other hand, since $\mathcal{G}$ is undirected, $w_{i,j} = w_{j,i}$.

Therefore, for all $v \in \mathbb{R}^n$,

$$\begin{aligned}
\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j}(v_i - v_j)^2 &= \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j}(v_i^2 + v_j^2 - 2v_iv_j) \\
&= \sum_{i=1}^{n} d_i v_i^2 - \sum_{i=1}^{n}\sum_{j=1}^{n} w_{i,j} v_i v_j \\
&= v^\top (D - W)v.
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\end{aligned}$$

The matrix $L := D - W$ is called the Laplacian matrix of the graph $\mathcal{G} = (V, W)$.

Spectral clustering

Coming back to the initial problem, we have relaxed the problem to

$$\underset{\substack{v^{(1)},\dots,v^{(K)}\\ \langle v^{(k)},Dv^{(k')}\rangle=\mathbf{1}_{k=k'}}}{\arg\min} \sum_{k=1}^{K}(v^{(k)})^\top L v^{(k)} = \underset{\substack{Y\in\mathbb{R}^{n\times K}\\ Y^\top DY=I_K}}{\arg\min} \operatorname{Tr}(Y^\top LY).$$

This is exactly the K smallest generalized eigenstructure $(y^{(1)}|\cdots|y^{(K)}) \in \mathbb{R}^{n\times K}$ of (L, D).

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– This algorithm called Spectral Clustering is widely used in clustering (Giulini 2016; Von Luxburg 2007).

– Because we solve a relaxation, the output $Y \in \mathbb{R}^{n\times K}$ is no longer a matrix of *hard* indicators (rows are not one-hot vectors). It should rather be interpreted as a *soft assignment*.

To recover a *discrete* partition, one applies a rounding step, such as

- **Thresholding:** $\hat{k}(i) \in \arg\max_{1\le k\le K} y_i^{(k)}$, and set $i \in \widehat{V}^{(\hat{k}(i))}$.
- **Euclidean clustering:** Apply k-means on the rows $\{y_i\}_{i=1}^{n}$ (often after normalization)

Laplacian Eigenmaps VS Spectral Clustering

$$\underset{\substack{Y \in \mathbb{R}^{n \times K} \\ Y^\top D Y = I_K}}{\arg\min} \ \operatorname{Tr}(Y^\top L Y).$$

For localized kernel graphs $w_{i,j} = k(\|x_i - x_j\|)$, this is Laplacian Eigenmaps with $K = d + 1$.

Laplacian Eigenmaps VS Spectral Clustering

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For localized kernel graphs $w_{i,j} = k(\|x_i - x_j\|)$, this is Laplacian Eigenmaps with $K = d + 1$.

The difference is the post-processing / interpretation:

- Spectral clustering does not drop the smallest eigenvalues, and you have to discretize the vectors (e.g. via k-means) to recover a partition.
- Laplacian eigenmaps uses eigenvectors as continuous coordinates.

Two regimes, one computation:

- If the kernel graph is *nearly disconnected* into K weakly linked regions, the first eigenvectors are *almost piecewise-constant* $\Rightarrow$ clustering.
- If the graph is *well connected*, they vary *smoothly* across vertices and capture only *global, low-frequency* structure rather than separating clusters. $\Rightarrow$ manifold coordinates.

Supervised dimension reduction

Discriminant Analysis

So far, we have addressed unsupervised data: all the coordinates of $x \in \mathbb{R}^p$ were considered in the same way.

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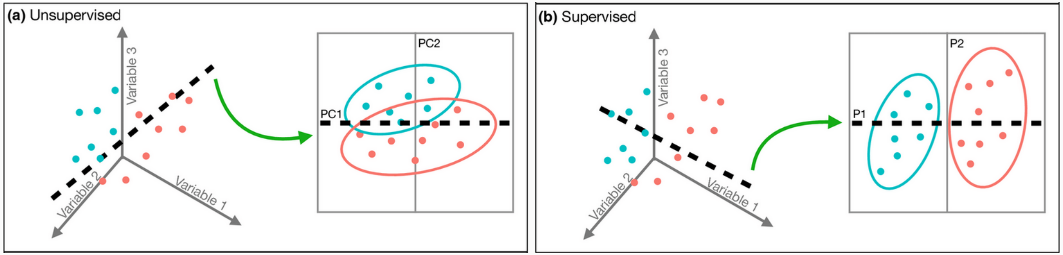
In supervised learning where groups of data points are known, one may wonder which variables contribute most to the geometric separation of some available labels.



Linear / Fisher discriminant analysis

Linear Discriminant Analysis, also called Fisher Discriminant Analysis, dates back to (Fisher 1936) on the `Iris` dataset.

Quoting Fisher, the method is meant to find the best

> *"linear functions of the measurements by which the populations are best discriminated"*

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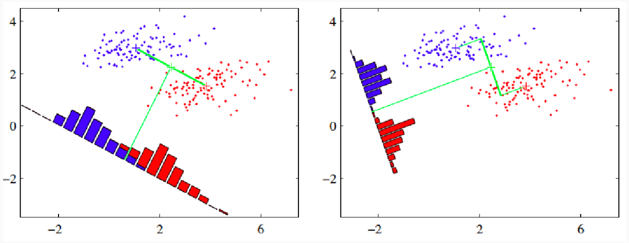
Idea: project while maximizing between-class variance *relative* to the within-class variance.



Total / Within-class / and Between-class variance

Write $(x, c) \in \mathbb{R}^p \times \{1, \ldots, J\}$ for the labeled data with J classes.

- The dataset has mean $\mu_T := \mathbb{E}_x[x]$ and total covariance

$$\mathbb{R}^{p\times p} \ni \Sigma_T := \mathbb{E}_x[(x-\mu_T)(x-\mu_T)^\top] = \frac{1}{n}\sum_{j=1}^{J}\sum_{i=1}^{n^{(j)}}(x_i^{(j)}-\mu_T)(x_i^{(j)}-\mu_T)^\top.$$

- Each class $j \in \{1, \ldots J\}$ has mean $\mu^{(j)} := \mathbb{E}_x[x \mid c = j]$ and within-class covariances

$$\mathbb{R}^{p\times p} \ni \Sigma_W^{(j)} := \mathbb{E}_x\left[(x-\mu^{(j)})(x-\mu^{(j)})^\top \mid c = j\right] = \frac{1}{n^{(j)}}\sum_{i=1}^{n^{(j)}}(x_i^{(j)}-\mu^{(j)})(x_i^{(j)}-\mu^{(j)})^\top.$$

- Across the classes, the between-class covariance is

$$\mathbb{R}^{p\times p} \ni \Sigma_B := \mathbb{E}_x\left[\left[(\mathbb{E}(x \mid c)-\mathbb{E}(x))(\mathbb{E}(x \mid c)-\mathbb{E}(x))^\top\right] = \frac{1}{n}\sum_{j=1}^{J} n^{(j)}(\mu^{(j)}-\mu_T)(\mu^{(j)}-\mu_T)^\top.$$

Linking the variances

Since

$$\mathbb{E}_x\left[(x - \mathbb{E}_x(x \mid c))(\mathbb{E}_x(x \mid c) - \mathbb{E}_x(x))^\top\right] = 0,$$

we get the decomposition

$$\begin{aligned}
\Sigma_T &= \mathbb{E}_x[(x - \mathbb{E}_x(x))(x - \mathbb{E}_x(x))^\top] \\
&= \mathbb{E}[(x - \mathbb{E}(x \mid c))(x - \mathbb{E}(x \mid c))^\top] + \mathbb{E}[(\mathbb{E}_x(x \mid c) - \mathbb{E}_x(x))(\mathbb{E}_x(x \mid c) - \mathbb{E}_x(x))^\top] \\
&= \Sigma_W + \Sigma_B,
\end{aligned}$$

where

$$\Sigma_W := \sum_{j=1}^{J} \frac{n^{(j)}}{n} \Sigma_W^{(j)} \qquad \text{and} \qquad \Sigma_B := \sum_{j=1}^{J} \frac{n^{(j)}}{n} (\mu^{(j)} - \mu_T)(\mu^{(j)} - \mu_T)^\top.$$

Linear Discriminant Analysis

Take a linear transformation (encoder) $A \in \mathbb{R}^{d \times p}$, and set $y_i := Ax_i$. Equivalently $Y := XA^\top$.

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- maximize the inertia of between-class distance $\mathrm{Cov}_B(Y) = A\Sigma_B A^\top$;
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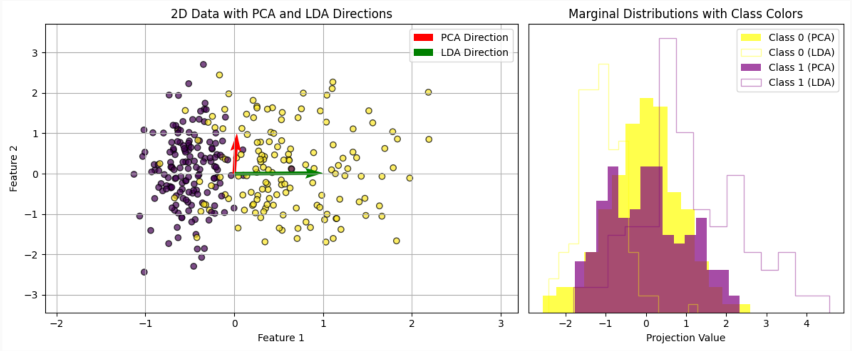
This leads to Linear Discriminant Analysis.

$$A_{\mathrm{LDA}} := \operatorname*{arg\,max}_{A\in\mathbb{R}^{d\times p}} \frac{\mathrm{Tr}(A\Sigma_B A^\top)}{\mathrm{Tr}(A\Sigma_W A^\top)},$$

with associated reduced point cloud $Y_{\mathrm{LDA}} := XA_{\mathrm{LDA}}^\top$.

PCA vs LDA

$$A_{\mathrm{PCA}} := \underset{A \in \mathbb{R}^{d \times p}}{\arg\max} \frac{\operatorname{Tr}(A \Sigma_T A^\top)}{\operatorname{Tr}(A A^\top)}, \qquad A_{\mathrm{LDA}} := \underset{A \in \mathbb{R}^{d \times p}}{\arg\max} \frac{\operatorname{Tr}(A \Sigma_B A^\top)}{\operatorname{Tr}(A \Sigma_W A^\top)}.$$



Compared to PCA, LDA increases the between-scatter and decreases the within-scatter.

Remarks

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– Many variants exist (Ghojogh et al. 2023).

– Can be seen as a classification algorithm with likelihood maximization (Kim, Magnani, and Boyd 2005).

– If Σ_W is (too close to being) singular, one may modify it and replace its smallest eigenvalues by a fixed user-defined value to robustify it (Deng et al. 2007; Guo and Wang 2015).

Fifty shades of linear discriminant component analysis

To account for unbalanced classes, one may also consider the same generalized eigenvalue problem with different scatter/covariance matrices.

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In Discriminative component analysis, (Hoi et al. 2006) take instead

$$\widetilde{\Sigma}'_B := \frac{1}{J(J-1)} \sum_{\ell=1}^{J} \sum_{j=1}^{J} (\mu^{(\ell)} - \mu^{(j)})(\mu^{(\ell)} - \mu^{(j)})^\top,$$

or

$$\widetilde{\Sigma}'_B := \frac{1}{J} \sum_{\ell=1}^{J} (\mu^{(\ell)} - \mu_T)(\mu^{(\ell)} - \mu_T)^\top ?$$

In Relevant Component analysis, (Shental et al. 2002) take instead

$$\widetilde{\Sigma}'_W = \frac{1}{nJ} \sum_{j=1}^{J} \sum_{i=1}^{n^{(j)}} (x_i^{(j)} - \mu^{(j)})(x_i^{(j)} - \mu^{(j)})^\top$$

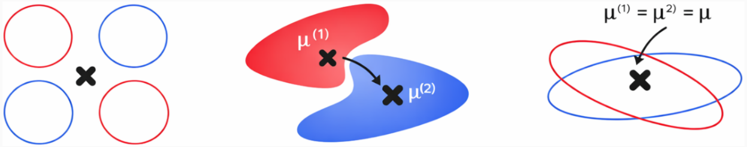
Limitations of LDA

Dimensionality bound. With J classes, LDA returns $J-1$ discriminant directions: If a classifier seems to require more than $J-1$ informative features, one must complement LDA with another representation.

Modeling assumption. LDA is somehow optimal under the simplistic generative picture

$$x \mid (Y=j) \;\approx\; \mathcal{N}(\mu^{(j)}, \Sigma) \quad \text{(one Gaussian per class, common covariance).}$$

When class-conditional distributions are far from Gaussian (multimodal, heavy-tailed, curved), the LDA projection can wash out this finer geometry.



LDA will also fail when the discriminatory information is not in the mean but rather in the variance of the data.

Featurized Component Analysis

Instead of minimizing a non-convex objective over a complicated hypothesis space, we may first apply a feature map

$$\Phi : \mathbb{R}^p \to \mathcal{H}$$

and then run LDA in feature space. Write $\widetilde{x}_i := \Phi(x_i) \in \mathcal{H}$ for the transformed variables.

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Denote by $\widetilde{\mu}^{(j)} := \mathbb{E}[\widetilde{x} \mid c = j], \widetilde{\mu}_T := \mathbb{E}[\widetilde{x}]$ the class and global means in $\mathcal{H}$.

Define the (feature-space) between/within covariances as linear operators $\mathcal{H} \to \mathcal{H}$:

$$\widetilde{\Sigma}_B := \sum_{j=1}^{J} \frac{n^{(j)}}{n} (\widetilde{\mu}^{(j)} - \widetilde{\mu}_T)^{\otimes 2}, \quad \widetilde{\Sigma}_W := \sum_{j=1}^{J} \frac{n^{(j)}}{n} \widetilde{\Sigma}_W^{(j)}, \quad \widetilde{\Sigma}_W^{(j)} := \mathbb{E}\left[(\widetilde{x} - \widetilde{\mu}^{(j)})^{\otimes 2} \mid c = j\right].$$

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Rayleigh quotient for feature-space LDA: for $a \in \mathcal{H} \setminus \{0\}$,

$$\mathcal{R}(a) := \frac{\langle a, \widetilde{\Sigma}_B a \rangle_{\mathcal{H}}}{\langle a, \widetilde{\Sigma}_W a \rangle_{\mathcal{H}}}.$$

Representer theorem: reduce the search to an n-dimensional span

We seek directions $a \in \mathcal{H}$ maximizing $\mathcal{R}(a)$. In finite sample, the relevant information lives in

$$\mathrm{span}\{\widetilde{x}_1, \ldots, \widetilde{x}_n\} \subset \mathcal{H}.$$

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Representer principle (finite-sample). For Fisher-type criteria built from empirical means/covariances, an optimizer can be chosen in the form

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Then the feature-space coordinate of point x_j becomes

$$y_j = \langle a, \widetilde{x}_j \rangle_{\mathcal{H}} = \sum_{i=1}^{n} \alpha_i \langle \widetilde{x}_i, \widetilde{x}_j \rangle_{\mathcal{H}} = (\mathbb{K}\alpha)_j, \qquad \mathbb{K}_{ij} := K(x_i, x_j).$$

Centering in feature space via Gram matrices

Most works assume centered features. In $\mathcal{H}$, centering amounts to replacing $\widetilde{x}_i$ by

$$\widetilde{x}_i^c := \widetilde{x}_i - \widetilde{\mu}_T.$$

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Define the centering matrix

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$$G := H\mathbb{K}H, \qquad G_{ij} = \langle \widetilde{x}_i^c, \widetilde{x}_j^c \rangle_{\mathcal{H}}.$$

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As for classical scaling, all inner products between centered linear combinations of $(\widetilde{x}_i)$ can be computed with G only.

Kernel LDA: class averaging operator and two Gram-only scatters

Let $c_i \in \{1, \dots, J\}$ be the label of x_i and set $n^{(j)} := |\{i : c_i = j\}|$.

Define the class-averaging matrix $M \in \mathbb{R}^{n \times n}$ by

$$M_{ij} := \begin{cases} \frac{1}{n^{(c_i)}} & \text{if } c_i = c_j, \\ 0 & \text{otherwise.} \end{cases} \qquad \Longrightarrow \qquad (Mv)_i = \frac{1}{n^{(c_i)}} \sum_{j : c_j = c_i} v_j .$$

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For a coefficient vector $\alpha \in \mathbb{R}^n$ and $y := G\alpha$ (centered), one checks the identities

$$\text{(between)} \quad \alpha^\top G(M - \tfrac{1}{n}\mathbf{1}\mathbf{1}^\top)G\,\alpha = \sum_{j=1}^{J} \frac{n^{(j)}}{n} \left(\bar{y}^{(j)} - \bar{y}_T\right)^{\otimes 2},$$

$$\text{(within)} \quad \alpha^\top G(I - M)G\,\alpha = \frac{1}{n} \sum_{j=1}^{J} \sum_{i : c_i = j} \left(y_i - \bar{y}^{(j)}\right)^{\otimes 2},$$

where $\bar{y}^{(j)}$ is the average within class j and $\bar{y}_T$ the global average.

Kernel LDA as a Rayleigh quotient in $\mathbb{R}^n$

We end up with the Gram-only Rayleigh quotient defined for all $\alpha \in \mathbb{R}^n$ by

$$\mathcal{R}(\alpha) := \frac{\alpha^\top G(M - \frac{1}{n}\mathbf{1}\mathbf{1}^\top)G\,\alpha}{\alpha^\top G(I - M)G\,\alpha}.$$

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A standard ridge-regularized kernel LDA direction solves

$$\alpha^\star \in \arg\max_{\alpha \neq 0} \frac{\alpha^\top G(M - \frac{1}{n}\mathbf{1}\mathbf{1}^\top)G\,\alpha}{\alpha^\top \big(G(I - M)G + \varepsilon I\big)\,\alpha}, \qquad \varepsilon > 0.$$

Equivalently, $\alpha^\star$ is a top generalized eigenvector of

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The embedded coordinate is $y = G\alpha^\star$, and multiple components come from multiple orthogonal eigenvectors. (as now usual at this point of the class!)

Multi-class dimension bound: still at most $J-1$ directions

Even in feature space, the between-class operator has rank at most $J-1$:

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Indeed, $\widetilde{\Sigma}_B$ is a sum of J rank-one operators built from $\widetilde{\mu}^{(j)} - \widetilde{\mu}_T$, but these J vectors satisfy

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Conclusion: Kernel LDA can yield at most $J-1$ non-trivial discriminant components (same limitation as LDA).

Supervised PCA: from HSIC to a Rayleigh quotient

Supervised PCA (Barshan et al. 2011) selects directions that *maximally correlate* to labels.

The so-called Hilbert-Schmidt Independence Criterion is $\mathrm{HSIC} := \frac{1}{(n-1)^2}\mathrm{Tr}\big(K_X H K_C H\big)$, with K_X and K_C Gram matrices on samples and H the centering matrix.

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If we restrict to *linear* projections $z = Xa$ (one component), take $K_X(a) := zz^\top = Xaa^\top X^\top$ and a fixed label-kernel K_C. Then

$$\mathrm{HSIC}(Xa, C) \propto \mathrm{Tr}\big((Xaa^\top X^\top)HK_CH\big) = a^\top X^\top HK_CHX\, a.$$

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The Rayleigh quotient for Supervised PCA is defined for all $a \in \mathbb{R}^p$ by

$$\mathcal{R}_{\mathrm{SPCA}}(a) := \frac{a^\top\big(X^\top HK_CHX\big)a}{a^\top(X^\top X)\,a}.$$

Supervised PCA: generalized eigenvectors

For multiple components $A \in \mathbb{R}^{d \times p}$, the natural trace form is

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Imposing the standard whitening constraint $A X^\top X A^\top = I_d$ gives

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$\hookrightarrow$ Compare with PCA: $X^\top X a = \lambda a$.

Overall correlation: fix notation and connect to HSIC

Given centered random variables $U \in \mathbb{R}^u$ and $V \in \mathbb{R}^v$, define their cross-covariance

$$\Sigma_{UV} := \mathbb{E}[UV^\top] \in \mathbb{R}^{u \times v}.$$

(Here $UV^\top$ is $u \times v$; not $U^\top V$.)

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The Hilbert–Schmidt norm (a.k.a. Frobenius norm) summarizes second-order dependence:

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HSIC is the nonlinear analogue: it replaces (U, V) by RKHS features and replaces covariances by RKHS covariance operators, whose Hilbert–Schmidt norm is computed from Gram matrices.

Robust Fisher Discriminant Analysis: worst-case Rayleigh quotient

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$\hookrightarrow$ Under convex uncertainty models, this becomes a tractable convex problem (often a regularized eigenproblem).

Quadratic Discriminant Analysis: generative model and decision rule

Quadratic Discriminant Analysis (QDA) uses a Gaussian model with class-dependent covariances:

$$x \mid (Y = j) \sim \mathcal{N}(\mu^{(j)}, \Sigma^{(j)}), \qquad j \in \{1, \dots, J\},$$

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The Bayes rule selects the class maximizing the log-posterior score

$$\delta_j(x) := -\frac{1}{2}(x - \mu^{(j)})^\top (\Sigma^{(j)})^{-1}(x - \mu^{(j)}) - \frac{1}{2}\log\det\Sigma^{(j)} + \log\pi_j.$$

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If all $\Sigma^{(j)}$ are equal, $\delta_j(x)$ is affine in x and we recover LDA. If not, the boundary $\delta_j(x) = \delta_{j'}(x)$ is quadratic in x.

Supervised dimension reduction with RKHS: the SDR principle

(Fukumizu, Bach, and Jordan 2004) studies sufficient dimension reduction (SDR): find $Z = \psi(X) \in \mathbb{R}^d$ such that

$$Y \perp\!\!\!\perp X \,\big|\, Z.$$

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Interpretation: Z keeps exactly the information in X that is useful to predict Y.

A convenient proxy is to minimize a conditional dependence measure:

$$Z \text{ is good} \quad \Longrightarrow \quad \text{“}\Sigma_{YY|Z} \text{ is small”}$$

where $\Sigma_{YY|Z}$ is a conditional covariance operator in an RKHS on Y.

RKHS view: conditional covariance operator and a Gram estimator

Let $\mathcal{H}_Y$ be an RKHS on $\mathcal{Y}$ and $\Phi_Y(Y) \in \mathcal{H}_Y$. Define the covariance operators

$$\Sigma_{YY} := \mathbb{E}\left[(\Phi_Y(Y) - \mu_Y) \otimes (\Phi_Y(Y) - \mu_Y)\right], \qquad \Sigma_{YZ} := \mathbb{E}\left[(\Phi_Y(Y) - \mu_Y) \otimes (\Phi_Z(Z) - \mu_Z)\right],$$

and similarly Σ_{ZZ}.

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$$\Sigma_{YY} := \mathbb{E}\left[(\Phi_Y(Y) - \mu_Y) \otimes (\Phi_Y(Y) - \mu_Y)\right], \qquad \Sigma_{YZ} := \mathbb{E}\left[(\Phi_Y(Y) - \mu_Y) \otimes (\Phi_Z(Z) - \mu_Z)\right],$$

and similarly Σ_{ZZ}.

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See (Fukumizu, Bach, and Jordan 2004) for the precise estimators and assumptions.

Neighborhood Components Analysis: a probabilistic kNN objective

Neighborhood Components Analysis (NCA) (Goldberger et al. 2004) learns a representation

$$z_i := Ax_i \in \mathbb{R}^d, \qquad A \in \mathbb{R}^{d \times p},$$

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Then the probability that x_i is correctly classified is

$$p_i(A) := \sum_{j:\ c_j = c_i} p_{ij}(A).$$

NCA maximizes

$$F(A) := \sum_{i=1}^{n} p_i(A) \qquad \text{or} \qquad G(A) := \sum_{i=1}^{n} \log p_i(A).$$

NCA: comparison with Rayleigh-quotient methods

Unlike PCA / LDA / kernel-LDA / supervised PCA, NCA is not a Rayleigh quotient.

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Heuristic: Rayleigh quotients optimize *global second-order structure*. NCA optimizes a *local classification* criterion (soft kNN).

Roweis Discriminant Analysis: a unifying Rayleigh template

Roweis Discriminant Analysis (RDA) (Ghojogh et al. 2023; Hoi et al. 2006) organizes many supervised DR methods as instances of

$$\operatorname*{arg\,max}_{A\in\mathbb{R}^{d\times p}} \frac{\mathrm{Tr}(A\,\Sigma_{\mathrm{num}}\,A^\top)}{\mathrm{Tr}(A\,\Sigma_{\mathrm{den}}\,A^\top)}.$$

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With a whitening constraint $A\Sigma_{\mathrm{den}}A^\top = I_d$, the solution is given by the top generalized eigenvectors of

$$\Sigma_{\mathrm{num}}a = \lambda\,\Sigma_{\mathrm{den}}a.$$

Double Supervised Discriminant Analysis: two uses of supervision

In the Roweis template, an extreme regime is to use supervision both in the numerator and in the normalization.

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Schematic form:

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Take-home: stronger supervision can yield sharper class separation, at the price of increased sensitivity to label noise / overfitting.

Large Margin Nearest Neighbor (LMNN): metric learning

A classical alternative to Fisher ratios is to learn a Mahalanobis metric

$$d_M(x, x')^2 := (x - x')^\top M (x - x'), \qquad M \succeq 0,$$

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LMNN solves a convex problem in M:

$$\min_{M\succeq 0} \sum_i \sum_{j\in\mathcal{N}_i} d_M(x_i,x_j)^2 + C \sum_i \sum_{j\in\mathcal{N}_i} \sum_{\ell:\ c_\ell\neq c_i} \left[1 + d_M(x_i,x_j)^2 - d_M(x_i,x_\ell)^2\right]_+ .$$

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