# Advanced course in machine learning
# 582744
# Lecture 7

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# Moodle

Moodle is open
`https://moodle.helsinki.fi/course/view.php?id=20396`

- I will announce exercises and their solutions here as news items – you get email notification for this (and hopefully can turn them of as well)
- One thread for each exercise, use to ask questions or clarifications and me and Aditya will reply as soon as we can
- Feel free to help other students, but do not give direct answers
- If you want to see something else in Moodle, just let us know

# Outline

# Supervised learning (from lecture 3)

The thing we all know:

- Input: $\mathbf{x}_n, y_n$
- Learning task: $f(\mathbf{x}_n) \approx y_n$
- Use: $f(\mathbf{x})$

# Linear regression

Minimize the squared loss

$$L(\mathbf{w}) = \sum_n (y_n - \mathbf{w}^T \mathbf{x}_n)^2$$

Solution using pseudo-inverse

$$\mathbf{w} = (\mathbf{X}\mathbf{X}^T)^{-1}\mathbf{X}\mathbf{y},$$

which is nothing but the solution for $\nabla L = 0$

Want bias term? Easiest to implement by adding $\mathbf{X}_{1n} = 1 \quad \forall n$ as the first element of the covariates

# Linear regression

Probabilistic formulation

$$p(y_n|\mathbf{w}, \mathbf{x}_n, \sigma^2) = N(\mathbf{w}^T\mathbf{x}_n, \sigma^2)$$

gives the negative log-likelihood

$$L(\mathbf{w}, \sigma^2) = C + \log \sigma^2 + \frac{1}{2\sigma^2} \sum_n (y_n - \mathbf{w}^T\mathbf{x}_n)^2$$

Irrespective of $\sigma^2$ we need to minimize the same squared loss, but we also get an estimate for the residual noise

$y_n$ can just as well be multivariate, making $\mathbf{w}$ a matrix. We simply model each dimension independently

# Linear regression vs PCA

The probabilistic models

$$\mathbf{y}_n \sim N(\mathbf{W}^T \mathbf{x}_n, \sigma^2 \mathbf{I}) \qquad \text{(LR)}$$

and

$$\mathbf{x}_n \sim N(\mathbf{W}^T \mathbf{z}_n, \sigma^2 \mathbf{I}) \qquad \text{(PCA)}$$

look awfully similar

One can think of PCA as linear regression where the covariates are unknown and need to be estimated as well

# Regularized linear regression

Even though linear regression is extremely simple model, it still overfits when the dimensionality is large compared to the amount of data – we already saw this in exercise 2

The prior $\mathbf{w}_d \sim N(0, \alpha)$ results in the log-loss

$$L(\mathbf{w}, \sigma^2) = C + \log \sigma^2 + \frac{1}{2\sigma^2} \sum_n (y_n - \mathbf{w}^T \mathbf{x}_n)^2 + \alpha \mathbf{w}^T \mathbf{w},$$

and after some elementary calculus we get the MAP solution

$$\mathbf{w} = (\mathbf{X}\mathbf{X}^T + \alpha \mathbf{I})^{-1} \mathbf{X}\mathbf{y}$$

This is called *ridge regression*, which has the effect of pulling the elements of $\mathbf{w}$ towards zero. Cross-validation can be used for choosing $\alpha$.

# Robust linear regression

What if we have outliers?

Student's t-distribution has heavier tails than normal distribution, and hence

$$y_n \sim t_\nu(\mathbf{w}^T \mathbf{x}_n, \sigma^2)$$

gives a more robust linear regression model

Laplace distribution $\log p \propto |y_n \mathbf{w}^T \mathbf{x}_n|$ would also work

No closed-form solution, so optimization is harder

# Logistic regression

Generalized linear models (Section 9; not covered on the course) are linear models that use other exponential family densities in place of the Gaussian likelihood

*Logistic regression* is one important special case:

$$p(y_n|\mathbf{w}, \mathbf{x}_n) = \text{Ber}(y|\text{sigm}(\mathbf{w}^T\mathbf{x}_n))$$

We already saw the negative log-likelihood in exercise 2.1, and even derived the gradient for minimizing it

In matrix-form the prettiest equations are probably

$$\mathbf{g} = \mathbf{X}^T(\boldsymbol{\mu} - \mathbf{y})$$
$$\mathbf{H} = \mathbf{X}^T\mathbf{S}\mathbf{X},$$

where $\boldsymbol{\mu}_n = \text{sigm}(\mathbf{w}^T\mathbf{x}_n)$ and $\mathbf{S} = \text{diag}(\boldsymbol{\mu}_n(1 - \boldsymbol{\mu}_n))$

# Logistic regression

Newton's method solves the problem well, and can be re-interpreted as *iteratively reweighted least squares* (IRLS) because it iteratively solves optimization problems of the form

$$L(\mathbf{w}) = \sum_n s_n (z_n - \mathbf{w}^T \mathbf{x}_n)^2$$

where $s_n$ are weights and $z_n$ are pseudo-targets (see Section 8.3.4)

Regularized version with the prior $\mathbf{w}_{nd} \sim N(0, \alpha)$ simply adds $2\alpha\mathbf{w}$ for the gradient and $2\alpha\mathbf{I}$ for the Hessian

The model can also be extended for multiple outputs, as *multinomial logistic regression*, using the likelihood

$$p(y_n = c|\mathbf{W}, \mathbf{x}_n) = \frac{e^{\mathbf{w}_c^T \mathbf{x}_n}}{\sum_j e^{\mathbf{w}_j^T \mathbf{x}_n}}$$

The updates are given in Section 8.3.7; these are a bit messy and the Hessian is huge

# Sparsity

Linear models overfit when $D$ is large compared to $N$; in extreme cases $D \gg N$, for example $D = 10,000$ genes used as covariates for $N = 100$ patients

...or because we expanded the feature space to get a non-linear variant

One intuitively effective way of regularizing the model for such cases is *feature selection*, which means using only a subset of the original $D$ dimensions in the model

Plenty of techniques for selecting them in advance, but here we consider approaches that directly learn *sparse* solutions, implicitly selecting the features

# Direct sparsity

Probabilistic formulation: Introduce new latent variables $\gamma_d \sim \text{Ber}(\theta)$ that tell whether a feature is being used or not, and infer $p(\gamma|D) \propto p(D|\gamma)p(\gamma)$

The prior is $p(\gamma) = \theta^{\|\gamma\|_0}(1-\theta)^{D-\|\gamma\|_0}$, where $\|\gamma\|_0$ is the $l_0$-norm that counts how many elemtents differ from zero

By further specifying that $\mathbf{w}_d = 0$ if $\gamma_d = 0$ and $\mathbf{w}_d \sim N(0, \alpha)$ if $\gamma_d = 1$, we can write a full probabilistic model

In the end it gives a regularization term $\lambda\|\gamma\|_0$

# Direct sparsity

Optimization for losses $L(\mathbf{w}) + \lambda \|\mathbf{w}\|_0$ is difficult because the regularizer is not smooth

- Greedy choice: Start with $\mathbf{w} = 0$ and always add the best dimension
- Backwards seletion: Start with $\gamma_d = 1 \quad \forall d$ and remove features greedily
- ...and a wide range of more advanced algorithms, including EM for a slightly modified prior

In practice we usually do not directly learn such a sparse model but try to find sparse models by other means

# Sparsity

The $l_2$ norm gave ridge regression that simply pulls the weights towards zero, whereas $l_0$ counted the number of non-zero elements and hence directly encorces sparsity

What if we tried regularizing with $l_p$ for some $0 \leq p \leq 2$, such as $l_1$?

Corresponds to the Laplace prior $e^{-\lambda \|w_d\|}$

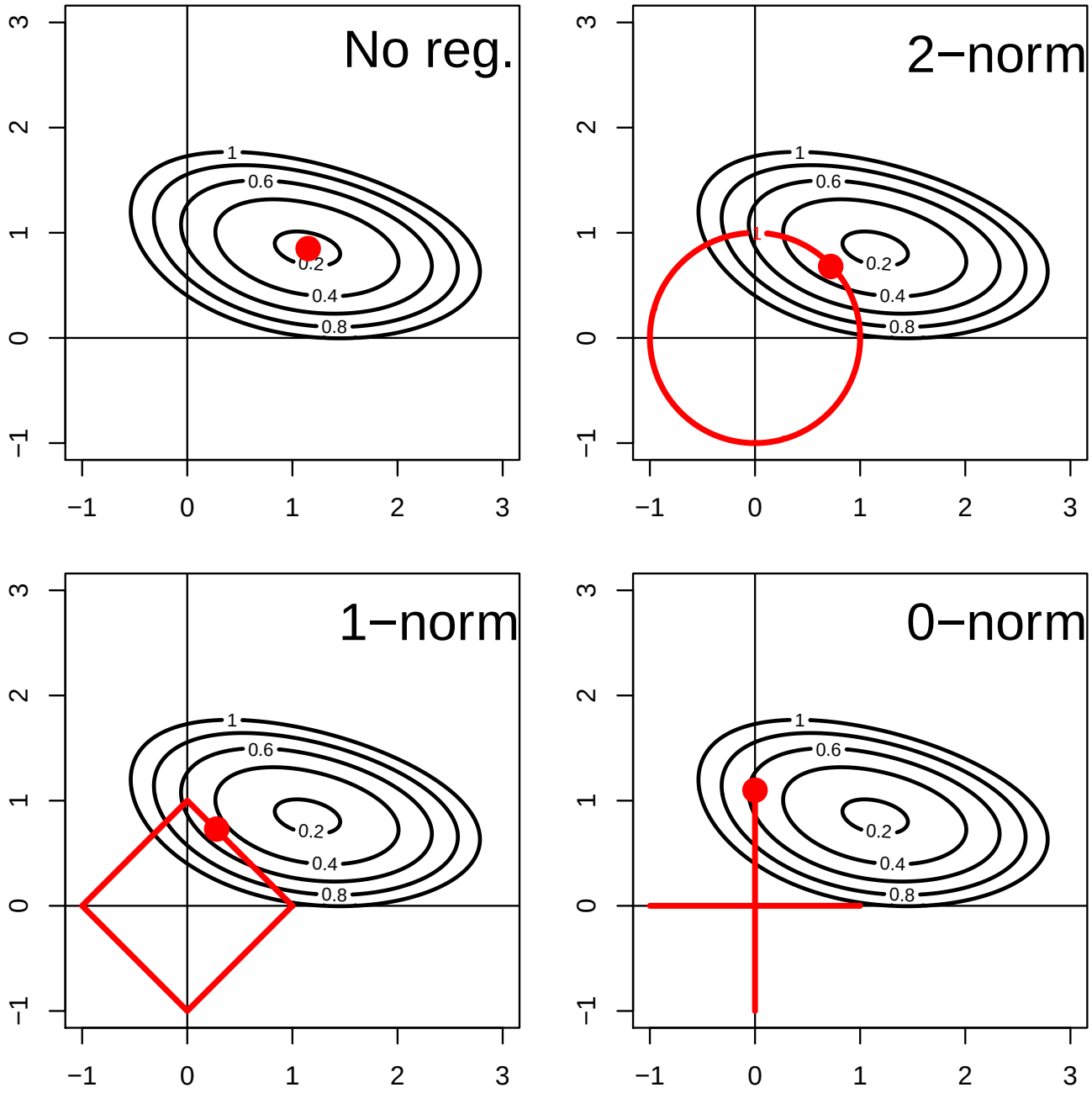
# Sparsity via regularization

Side-remark:
Minimizing $L(\mathbf{w}) + \lambda R(\mathbf{w})$ is equivalent to minimizing $L(\mathbf{w})$ such that $R(\mathbf{w}) \leq B$ for some $B$, where smaller $B$ correspond to larger $\lambda$

Might help geometric intuition: Regularized solution has to stay within a "ball" of given norm

...but the relationship between $B$ and $\lambda$ above depends on the data

# Sparsity – geometric motivation



# Sparse linear regression

Regression with $l_1$ regularization is called *lasso* for "least absolute shrinkage and selection operator"

$$L(\mathbf{w}) = \sum_n (y_n - \mathbf{w}^T \mathbf{x}_n)^2 + \lambda \|\mathbf{w}\|_1$$

The partial derivative of the regularizer is not defined at $\mathbf{w}_d = 0$, but we can use *subgradient* which is any slope that touches the loss function at such discontinuity and is below the curve

We find the minimum by following the subgradients, and for the solution the zero vector belongs to the family of subgradients

# Lasso (Section 13.3.2)

The full subgradient is given by

$$\nabla L(\mathbf{w}) = \begin{cases} a_d \mathbf{w}_d - c_d - \lambda & \text{if} \quad w_d < 0 \\ [-c_d - \lambda, -c_d + \lambda] & \text{if} \quad w_d = 0 \\ a_d \mathbf{w}_d - c_d + \lambda & \text{if} \quad w_d > 0, \end{cases}$$

where $a_d = 2 \sum \mathbf{X}_{nd}^2$ and $c_d = 2 \sum_n \mathbf{X}_{nd} (y_n - \mathbf{w}_{-d}^T \mathbf{X}_{n,-d})$

...and by setting it to zero we get the solution as

$$\begin{aligned} \mathbf{w}_d &= (c_d + \lambda)/a_d && \text{if} \quad c_d < -\lambda \\ \mathbf{w}_d &= 0 && \text{if} \quad c_d \in [-\lambda, \lambda] \\ \mathbf{w}_d &= (c_d - \lambda)/a_d && \text{if} \quad c_d > \lambda \end{aligned}$$

Pulls all weights towards zero by a constant amount, setting them exactly to zero if close enough

Compare to $l_2$ which divides the weights by $1 + \lambda$ (Section 13.5.3)

# Lasso

An algorithm called LARS ("least angle regression and shrinkage") can compute the solution for all values of $\lambda$ in roughly the same time as it takes to solve the problem for one value

Based on the observation that the set of non-zero values changes only for certain critical values of $\lambda$ and otherwise the weights change linearly

# $l_1$ algorithms

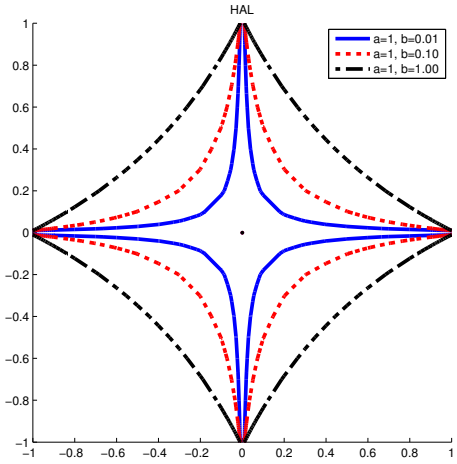
Optimization algorithm for general loss functions (such as logistic regression):

- Coordinate descent: Optimize over each dimension independently (the equations above actually did this)
- Proximal methods: For any combination of smooth convex loss function and non-smooth (but convex) regularizer
- Basic idea: Replace the non-smooth loss $R(\mathbf{w})$ with its proximal operator $\min_{\mathbf{z}} R(\mathbf{z}) + \|\mathbf{z} - \mathbf{w}\|^2$, giving a quadratic approximation for the regularized loss
- EM, after representing the Laplace distribution as Gaussian scale mixture (Section 13.4.4)

On this course knowing the first approach is enough

# Other sparsity priors

- Group-lasso: $l_1$-norm for groups of variables
- Elastic net: Sum of $l_2$ and $l_1$
- Bridge: $\sum_d \|w_d\|^b$ for $b \geq 0$ (note that $b = 1$ is the smallest one that is convex)
- Automatic relevance determination (ARD): $w_d \sim N(0, \alpha)$, with some flat prior for $\alpha$ (often used with PCA)



# Generative classifiers

The above models are *discriminative classifiers* since they directly optimize for a loss that is related to the output variable (that is, they model the conditional density $p(y|\mathbf{x})$)

An alternative is to consider *generative classifiers* that construct a model for the joint density $p(y, \mathbf{x})$ and use it to infer the conditional density

$$p(y|\mathbf{x}) = \frac{p(y, \mathbf{x})}{p(\mathbf{x})}$$

# Generative vs discriminative (Section 8.6.1)

- Generative often easier to fit
- ...but we are fitting a more complex representation
- Missing inputs easier for generative models
- Unlabeled examples can help for generative models (semi-supervised learning)
- Discriminative models support arbitrary preprocessing steps for the inputs
- Generative models rely more on the assumptions of the model

# Gaussian discriminant analysis

One practical generative classifier assumes $p(\mathbf{x}|y = c) = N(\mu_c, \Sigma_c)$

New samples classified using

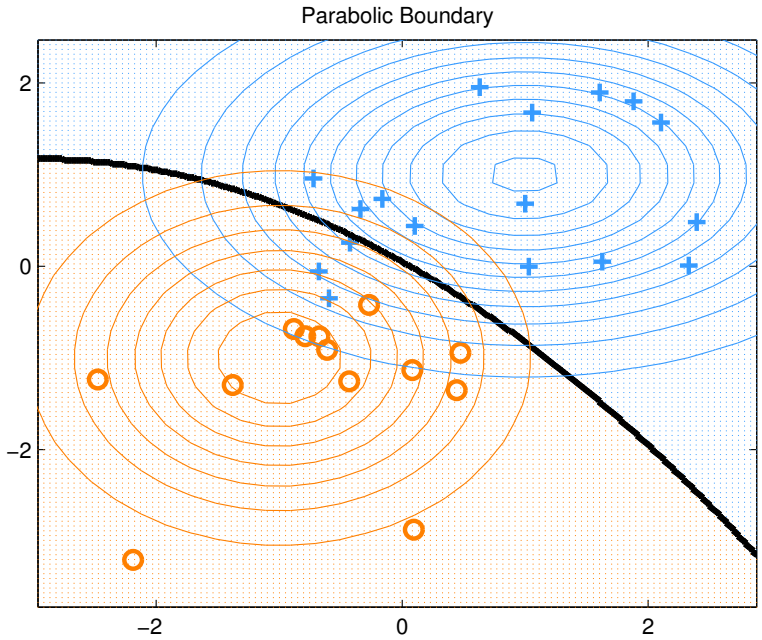
$$\arg\min(\mathbf{x} - \mu_c)^T \Sigma_c^{-1} (\mathbf{x} - \mu_c),$$

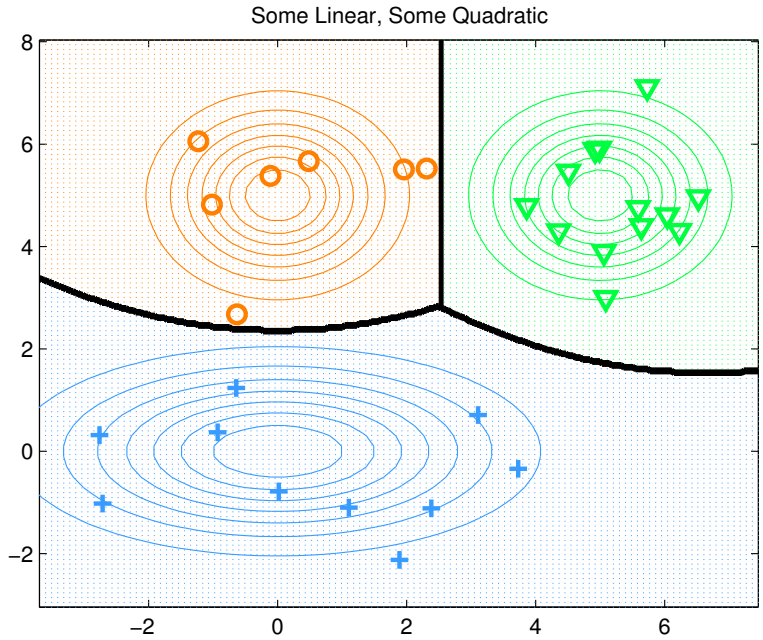
or by normalizing these to get the full posterior

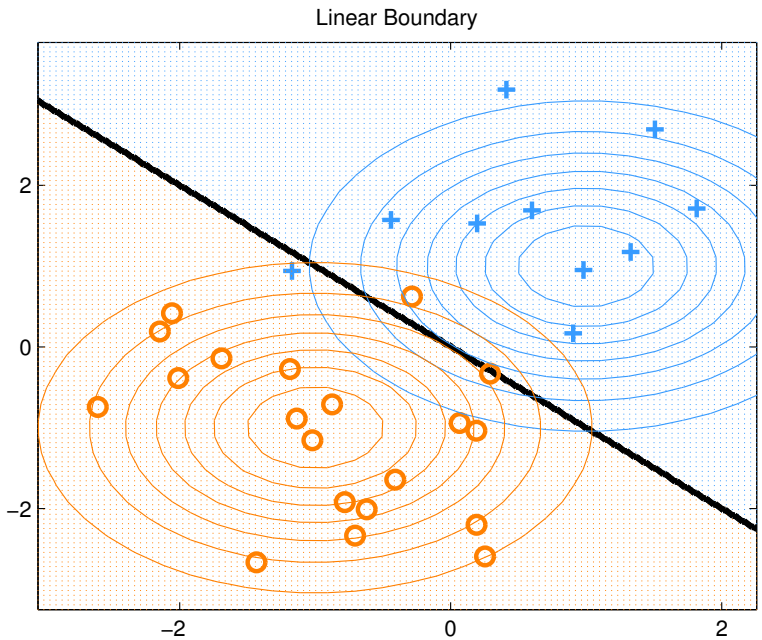
If the covariances are shared ($\Sigma_c = \Sigma$), we get *Linear discriminant analysis* (LDA), since the discriminative boundary becomes linear

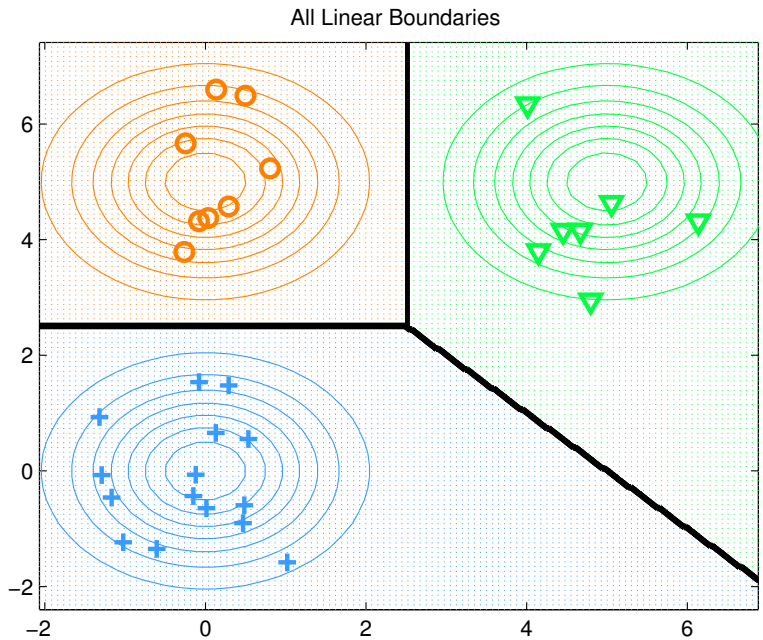
With general covariances the method is called *Quadratic discriminant analysis*

# Generative classifiers



# Mixtures of experts

We already saw how to create mixtures of PCAs

How about discriminative mixtures? Associate with each mixture component a discriminative model $p(y|\mathbf{x}_n)$

*Mixture of experts* combines a *gating network* that assigns samples into $K$ mixture components based on $\mathbf{x}$ alone with $K$ discriminative models for predicting $y$

$$p(y_n|\mathbf{x}_n, z_n = k, \boldsymbol{\theta}) = N(\mathbf{w}_k^T \mathbf{x}_n, \sigma_k^2)$$

$$p(z_n = k) \propto e^{\mathbf{v_k}^T \mathbf{x}_n}$$

# Mixture of experts