Variance inflation

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"Deep" network for decoding PET brain scans (1994)


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Variance inflation in
PCA
kPCA
Linear regression and SVMs

D sensors
N samples

D >> N
"HDLSS" high dimension, low sample size (Hall 2005, Ahn et al, 2007)
"Large p, small n" (West, 2003), "Curse of dimensionality" (Occam, 1350)
"Large underdetermined systems" (Donoho, 2001)
"Ill-posed data sets" (Kjems, Strother, LKH, 2001)
Factor models

Represent a datamatrix by a low-dimensional approximation

\[ X(i,t) \approx \sum_{k=1}^{K} A(i,k)S(k,t) \]
Unsupervised learning:
Factor analysis generative model

\[ x = As + \epsilon, \quad \epsilon \sim N(0, \Sigma) \]

\[
p(x | A, \theta) = \int p(x | A, s, \Sigma) p(s | \theta) ds
\]

\[
p(x | A, s, \Sigma) = \sqrt{2\pi\Sigma}^{-1/2} e^{-\frac{1}{2}(x-As)^T \Sigma^{-1} (x-As)}
\]

Source distribution:
PCA: ... normal
ICA: ... other
IFA: ... Gauss. Mixt.
kMeans: .. binary

PCA: \[ \Sigma = \sigma^2 \cdot 1 \]
FA: \[ \Sigma = D \]

S known: GLM
(1-A)\(^{-1}\) sparse: SEM
S,A positive: NMF

Højen-Sørensen, Winther, Hansen,
Neural Computation (2002),
Neurocomputing (2002)
Learning the parts of objects by non-negative matrix factorization

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Generalizability

- Generalizability is defined as *the expected performance on a random new sample*
  - A model's mean performance on a "fresh" data set is an unbiased estimate of generalization

- Typical loss functions:

\[
\langle -\log p(s \mid x, D) \rangle, \quad \langle -\log p(x \mid D) \rangle, \\
\langle (s - \hat{s}(D))^2 \rangle, \quad \log \frac{p(s, x \mid D)}{p(s \mid D)p(x \mid D)}
\]

- Results can be presented as "bias-variance trade-off curves" or "learning curves"

Bias-variance trade-off as function of PCA dimension in fMRI data

A Cure for Variance Inflation in High Dimensional Kernel Principal Component Analysis

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Variance inflation in PCA

Who shrunk the test set?
Modeling the generalizability of SVD

- Rich physics literature on “retarded” learning

- **Universality**
  - Generalization for a “single symmetry breaking direction” is a function of ratio of N/D and signal to noise S
  - For subspace models-- a bit more complicated -- depends on the component SNR’s and eigenvalue separation
  - For a single direction, the mean squared overlap $R^2 = \langle (u_1^T u_0)^2 \rangle$ is computed for $N,D \rightarrow \infty$

$$R^2 = \begin{cases} 
(\alpha S^2 - 1) / S(1 + \alpha S) & \alpha > 1 / S^2 \\
0 & \alpha \leq 1 / S^2 
\end{cases}$$

$$\alpha = N / D \quad S = 1 / \sigma^2 \quad N_c = D / S^2$$


$N_c = (0.0001, 0.2, 2, 9, 27, 64, 128, 234, 400, 625)$

$\sigma = (0.01, 0.06, 0.12, 0.17, 0.23, 0.28, 0.34, 0.39, 0.45, 0.5)$
Restoring the generalizability of SVD

• Now what happens if you are on the slope of generalization, i.e., N/D is just beyond the transition to retarded learning?

• The estimated projection is offset, hence, future projections will be too small!

• ...problem if discriminant is optimized for unbalanced classes in the training data!
Heuristic: Leave-one-out re-scaling of SVD test projections

Kjems, Hansen, Strother: “Generalizable SVD for Ill-posed data sets” NIPS (2001)

N=72, D=2.5 \times 10^4
Re-scaling the component variances by leave one out

Possible to compute the new scales by leave-one-out doing $N$ SVD’s of size $N << D$
Let \( \{x_1, \ldots, x_N\} \) be \( N \) training data points in a \( D \) dimensional input space

\[
x_N = x^\perp_N + x^\parallel_N,
\]

\[
u^T_{N-1,k} \cdot x_N = u^T_{N-1,k} \cdot x^\parallel_N,
\]

\[
u^T_{N-1,k} \cdot x_N = u^T_{N-1,k} \cdot x^\parallel_N \approx u^T_{N,k} \cdot x^\parallel_N
\]

Two approximations

Adjusting for the mean overlap

\[ R^2 = \begin{cases} 
\frac{(\alpha S^2 - 1)}{S(1 + \alpha S)} & \alpha > 1 / S^2 \\
0 & \alpha \leq 1 / S^2 
\end{cases} \]

\[ \alpha = \frac{N}{D} \quad S = \frac{1}{\sigma^2} \quad N_c = \frac{D}{S^2} \]


Adjusting for lost projection

\[ u_{N-1,k}^T \cdot x_N = u_{N-1,k}^T \cdot x_N \approx u_{N,k}^T \cdot x_N \]
Approximating the leave-one-out (LOO) procedure. Here we simulate data with four normal independent signal components, \( \mathbf{x} = \sum_{k=1}^{4} \eta_k \mathbf{u}_k + \mathbf{\epsilon} \) of strengths (1.4, 1.2, 1.0, 0.8), embedded in i.i.d. normal noise \( \mathbf{\epsilon} \sim N(0, \sigma^2 \mathbf{1}) \), with \( \sigma = 0.2 \). The dimension was \( D = 2000 \) and the sample size was \( N = 50 \). In the four panels we show the training set projections (red crosses), the projections corrected for the theoretical mean overlap (Hoyle and Rattray, 2007) (yellow squares) and the geometric approximation in Equation (1) (green dots) versus the exact LOO projections (black line).
Universality in PCA, NMF, Kmeans

- Looking for universality by simulation
  - learning two clusters in white noise.

- Train \( K=2 \) component factor models.

- Measure overlap between line of sight and plane spanned by the two factors.

**Experiment**

- **Variable:** \( N, D \)
- **Fixed:** SNR
Beyond the linear model:
Non-linear denoising and manifold representations

Beyond the linear model:

Kernel PCA is based on non-linear mapping of N data points

\[ x_n \rightarrow \varphi(x_n) \equiv \varphi_n \]

Our aim is to let the local geometry of mapped points represent the local geometry of the input space, hence we connect the spaces by the letting inner products be defined so that close points in input space are represented by high values of their inner product

\[ K_{n,n'} = \varphi_n^T \varphi_{n'} = \exp \left( - \frac{\|x_n - x_{n'}\|^2}{c} \right) \]

Note \( c \to \infty \) defaults to linear PCA

Beyond the linear model:

- Kernel PCA is based on non-linear mapping of data to

\[ x_n \rightarrow \varphi(x_n) \equiv \varphi_n, \quad n = 1, \ldots, N \]

Aim is to locate maximum variance directions in the feature space, i.e.

\[ l_1 \equiv \arg \max_{\|l\|=1} \left\langle \left( l^T \cdot \varphi \right)^2 \right\rangle, \quad \varphi(x_n) = \sum_k l_k s_{k,n} \]

The principal direction is in the span of data:

\[ l_1 = \sum_{n=1}^{N} a_{1,n} \varphi_n \]

\[ a_1 = \arg \max_{\|a\|=1} \left\langle a^T \cdot K \cdot a \right\rangle, \quad K_{n,n'} = \varphi_n^T \cdot \varphi_n' = \exp \left( -\frac{\|x_n - x_n'\|^2}{2c} \right) \]

Approximating the LOO cure for kPCA

Let \( \{x_1, \ldots, x_N\} \) be \( N \) training data points

\[
\tilde{\phi}(x) = \phi(x) - \bar{\phi}.
\]

\[
\tilde{K} = K - \frac{1}{N} 1_{NN} K - \frac{1}{N} K 1_{NN} + \frac{1}{N^2} 1_{NN} K 1_{NN}
\]

\[
\tilde{K} \alpha_i = \lambda_i \alpha_i
\]

\[
\beta_i = \tilde{\phi}(x)^T \nu_i = \sum_{n=1}^{N} \alpha_{in} \tilde{\phi}(x)^T \tilde{\phi}(x_n) = \sum_{n=1}^{N} \alpha_{in} \tilde{k}(x, x_n)
\]
\[ \| \mathbf{x}_n - \mathbf{x}_N \|^2 = \| \mathbf{x}_n - \mathbf{x}_N \|^2 + \| \mathbf{x}_N \|^2 \]

\[
\beta_i(\mathbf{x}_N) = \sum_{n=1}^{N-1} \alpha_{in} \tilde{k}(\mathbf{x}_N, \mathbf{x}_n) = \exp \left( -\frac{1}{c} \| \mathbf{x}_N \|^2 \right) \sum_{n=1}^{N-1} \alpha_{in} \tilde{k}(\mathbf{x}_N, \mathbf{x}_n)
\]
Application to classification of high-dimensional data on manifolds
Non-parametric histogram equalization

\[
\begin{align*}
\texttt{[as,ia]} &= \text{sort}(a); \\
\texttt{[bs,ib]} &= \text{sort}(b); \\
\texttt{b(ib)} &= \text{as};
\end{align*}
\]
Non-parametric histogram equalization

Algorithm 1: Approximate renormalization in kernel PCA

Require: $X_{tr}$ and $X_{te}$ to be $N_{tr} \times D$ and $N_{te} \times D$ respectively.

Compute $K_{tr}$ using Equation (2) and find the eigenvectors, $\alpha_1, \ldots, \alpha_q$.

for $i = 1$ to $N_{tr}$ do
    $f_{tr}^{i} \leftarrow P_q(x_{tr}^i) = \tilde{K}_{x1}^T \alpha^i q$ (see Equation (3))
end for

for $j = 1$ to $N_{te}$ do
    $f_{te}^{j} \leftarrow P_q(x_{te}^j) = \tilde{K}_{x1}^T \alpha^i q$ (see Equation (3))
end for

for $d = 1$ to $q$ do
    $[f_{sort}, J] \leftarrow \text{sort}(f_{tr}^{i:d})$ (ascending order)
    $[\cdot, I] \leftarrow \text{sort}(f_{te}^{j:d})$ (ascending order)
    if $N_{tr} = N_{te}$ then
        $h \leftarrow f_{sort}$
    else
        $h \leftarrow \text{spline}([1 : N_{tr}], f_{sort}, \text{linspace}(1, N_{tr}, N_{te}))$ (interpolate to create $N_{te}$ values of $f_{sort}$ in the interval $[1 : N_{tr}]$)
    end if
    for $n = 1$ to $N_{te}$ do
        $g_{te}^{i(n),d} \leftarrow h^{n,d}$ (renormalized test data in the principal subspace, see Equation (4))
    end for
end for
Application to classification of high-dimensional data on manifolds

Test prior to scaling

Test post scaling
Supervised learning from small samples in high dimensional spaces
EEG imaging

Linear ill-posed inverse problem

\[ Y: \ 1 \times N \]
\[ W: \ 1 \times D \]
\[ X: \ D \times N \]

\[ D \gg N \]

Need priors to solve!

Why 3D real-time imaging?

Enable on-line visual quality control

Neuro-feedback applications can be based on activity in specific brain structures/networks

Context priors may relate to 3D location (from meta analysis)

Evidence that BCI/decoding can be improved by 3D representation


Do we get meaningful 3D reconstructions?

Imagined finger tapping
Left or right cued (at t=0)

Signal collected from an AAL region

Meier, Jeffrey D., Tyson N. Aflalo, Sabine Kastner, and Michael SA Graziano.
Variance inflation in linear regression

\[ y = \mathbf{w}^\top \mathbf{x} + \epsilon = \sum_{d=1}^{D} w_d x_d + \epsilon \]

\[ \hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \sum_{n=1}^{N} (y_n - \mathbf{w}^\top \mathbf{x}_n)^2 \]

\[ G(N) = E_{y,\mathbf{x}} \left\{ E_{\mathbf{N}} \left\{ (y - \mathbf{w}_N^\top \mathbf{x})^2 \right\} \right\} \]

\[ G(N) = \begin{cases} 
(1 - \frac{N}{D}) \|\mathbf{w}_0\|^2 + \frac{D-1}{D-N-1} \sigma^2 & N < D - 1, \\
\infty & D - 1 \leq N \leq D + 1 \\
\frac{N-1}{N-D-1} \sigma^2 & N > D + 1.
\end{cases} \]

Fig. 1. Experimental and theoretical learning curves for the case \( D = 20 \) with \( \sigma^2 = 0.1, \|\mathbf{w}_0\|^2 = 1 \). The theoretical result for \( N > D + 1 \) is given in Hansen (1993). The sample size for the minimal error (for \( N < D - 1 \)) is located at \( N_{\text{min}} = |D - 1 - \sqrt{D(D-1)} \sqrt{\frac{\sigma^2}{\|\mathbf{w}_0\|^2}}| = 13 \). The results are based on 10000 simulated data sets.


Variance inflation in linear regression

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\[ \|w_0\|^2 - E_N \left\{ \|\hat{w}\|^2 \right\} = \left(1 - \frac{N}{D}\right) \|w_0\|^2 \]
Variance inflation in linear regression

\[ \mathbf{w} = \sum_{n=1}^{N} \beta_{n} \mathbf{x}_{n} \quad K_{m,n} = \mathbf{x}_{m}^{\top} \mathbf{x}_{n} \]

\[ \mathbf{\hat{w}} = \sum_{m,n=1}^{N} \mathbf{x}_{n} (K^{-1})_{n,m} y_{m} \]

\[ \sigma^{2} \left( \mathbf{\hat{w}}^{\top} \mathbf{x}_{n} \right) = \frac{1}{N} \sum_{n=1}^{N} y_{n}^{2} \]

Training set variance of predictions

\[ E_{N} \left\{ \frac{1}{N} \sum_{n=1}^{N} y_{n}^{2} \right\} = \| \mathbf{w}_{0} \|^{2} + \sigma^{2} \]

Test set variance of predictions

\[ E_{x} \left\{ E_{N} \left\{ \mathbf{\hat{w}}^{\top} \mathbf{x} \right\} \right\} = E_{N} \left\{ \| \mathbf{\hat{w}} \|^{2} \right\} = \frac{N}{D} \| \mathbf{w}_{0} \|^{2} \]
Application to classification of high-dimensional data on manifolds
USPS data classification: Digit “8” vs rest

Test prior to scaling

Test post scaling
Functional MRI

- Indirect measure of neural activity - hemodynamics
- A cloudy window to the human brain

Challenges:
- Signals are multi-dimensional mixtures
- No simple relation between measures and brain state - “what is signal and what is noise”?

\[ TR = 333 \text{ ms} \]
Multivariate neuroimaging models

Neuroimaging aims at extracting the mutual information between stimulus and response.

- **Stimulus**: Macroscopic variables, ”design matrix” ... \( s(t) \)

- **Response**: Micro/meso-scopic variables, the neuroimage ... \( x(t) \)

- Mutual information is stored in the joint distribution ... \( p(x,s) \).

*Often \( s(t) \) is assumed known...unsupervised methods consider \( s(t) \) or parts of \( s(t) \) ”hidden”....*
Application to classification of high-dimensional data on manifolds (fMRI, exceptional good SNR in raw data)

Figure 11: Mean error rates ± 1 standard deviation as a function of the noise level for fMRI data ($D = 16,384, N = 605$). The test error based on conventional kernel PCA projections, renormalized projections, and a LOOCV scheme is shown. Renormalization is seen to clearly improve the performance. Arrow 'A' indicates the noise level used in Figure 12.
Application to classification of high-dimensional data on manifolds (fMRI, exceptional good SNR in raw data)

Figure 12: Test set projections of the fMRI data with Gaussian noise added as marked on Figure 11 ($\varepsilon_i = \mathcal{N}(0, 3.8^2)$). The top row shows the conventional projections, while the bottom row shows the projections after renormalization. The ‘red class’ indicates activation, while the blue observations are acquired during rest. The dashed line marks the linear discriminant. The scale is chosen as the 5th percentile of the mutual distances.
Implications for the SVM?

Distribution of the decision function

\[
\text{sign}(y(x)) = \text{sign}\left(\sum_{i \in S} y_i \alpha_i k(x_i, x) + b\right),
\]

\[
\beta_i(x_N) = \sum_{n=1}^{N-1} \alpha_{in} \tilde{k}(x_N, x_n) = \exp\left(-\frac{1}{c} \|x_N\|_2^2\right) \sum_{n=1}^{N-1} \alpha_{in} \tilde{k}(x_N, x_n)
\]

‘… unlike other machine learning methods, SVMs generalization error is related not to the input dimensionality of the problem, but to the margin with which it separates the data…’

J. Kwok IEEE TNN (1999)
Variance inflation in SVM decision function

Figure 1: Illustration of the variance inflation phenomena in simulated data. The plots show the distribution of the decision values, $f$, of a FLD. The top panel is the training data, the middle panel is the test data, and the lower panel shows the result after applying the non-parametric scheme for restoring the variation as described in following section. The inflated variance of the training data compared to the test data is evident.
Decision function mis-match in the SVM (USPS)

\[
G\text{-mean} = \sqrt{\text{sensitivity} \cdot \text{specificity}}
\]

![Graphs showing accuracy and G-mean as a function of noise level.](image)

**Fig. 1.** Mean performance measures ±1 std as a function of the noise level for the USPS data. The left and middle panels show the accuracy and the G-mean respectively. The test accuracy is shown in red while the renormalized test accuracy is shown in gray. The right panel shows an example of the histogram before and after renormalization (for a noise level of \(\sigma = 0.27\)).

T.J. Abrahamsen, LKH: Restoring the Generalizability of SVM based Decoding in High Dimensional Neuroimage Data
NIPS Workshop: Machine Learning and Interpretation in Neuroimaging (MLINI-2011)
Fig. 2. Mean performance measures ±1 std as a function of kernel hyperparameter for the fMRI data. Higher values of $\gamma$ lead to more non-linear kernel embeddings. The left and right panel shows the accuracy and the G-mean respectively. The dashed lines correspond to the scheme where data with no stimuli are omitted, while the full lines show the performance on the subsampled data. The test accuracy is shown in red while the renormalized test accuracy is shown in gray. The black crosses indicate the optimal kernel hyperparameter. Renormalization is seen to improve performance and notably it leads to more non-linear optimal kernels as the optimal scale parameters chosen by cross-validation are increased.
Conclusion

- Variance inflation in PCA
  Cure: Rescale std’s

- Variance inflation in kPCA
  Cure: Non-parametric renormalization of components

- Support Vector Machines:
  In-line renormalization seems to enable more non-linear classifiers in $D \gg N$
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