Nonlinear Forecasting with Many Predictors using Kernel Ridge Regression

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New Directions for Forecasting

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Main research question:

Is it possible to forecast with large data sets, while allowing for nonlinear relations between target variable and predictors?

Background:

Large data sets are increasingly available in macroeconomics and finance, but forecasting is mostly limited to a linear framework.

Solution:

Kernel ridge regression (KRR), which avoids the curse of dimensionality by manipulating the forecast equation in a clever way: the kernel trick.

Contributions:

- Extension of KRR to models with "preferred" predictors
- Monte Carlo and empirical evidence that KRR works, and improves upon conventional techniques such as principal component regression
- Clearer understanding of the choice of kernel and tuning parameters (companion paper)

Joint work with Patrick Groenen, Christiaan Heij, and Dick van Dijk (Econometric Institute, Erasmus University Rotterdam)
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In an ideal world:
- use all available information
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In practice:
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- Handling high-dimensionality:
  - Principal components regression (Stock and Watson, 2002)
  - Partial least squares (Groen and Kapetanios, 2008)
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  - Bayesian regression (De Mol, Giannone, Reichlin, 2008)

- Handling nonlinearity:
  - Neural networks (Ter¨ asvirta, Van Dijk, Medeiros, 2005)
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We aim to forecast \( y^* \in \mathbb{R} \), using a set of predictors \( x^* \in \mathbb{R}^N \).

Historical observations are collected in \( y \in \mathbb{R}^T \) and \( X \in \mathbb{R}^{T \times N} \).

Assuming a linear relation, we would use OLS to minimize
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||y - X\beta||^2
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Forecast would be \( \hat{y}^* = x^*\beta = x^* (X'X)^{-1}X'y \).

This requires \( N \leq T \) (in theory) or \( N \ll T \) (in practice).
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Ridge regression

A standard solution is ridge regression: given some $\lambda > 0$, minimize $\|y - X\beta\|^2 + \lambda \|\beta\|^2$. Even if $N > T$.

For very large $M$, the inversion is numerically unstable and computationally intensive. Typical example: $N = 132$, quadratic model $\Rightarrow M = 8911$. 

Peter Exterkate (CREATES, Aarhus University)
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- So, for nonlinear forecasts, let $z = \varphi(x)$ with $\varphi: \mathbb{R}^N \to \mathbb{R}^M$, and $\hat{y}_* = z_*'(Z'Z + \lambda I)^{-1}Z'y$
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- We wish to compute $\hat{y}_* = z'_* (Z'Z + \lambda I)^{-1} Z'y$

Some algebra yields $\hat{y}_* = z'_* Z'(ZZ' + \lambda I)^{-1} y$

So if we know $k_* = Zz'_* \in \mathbb{R}^T$ and $K = ZZ' \in \mathbb{R}^{T \times T}$, computing $\hat{y}_* = k'_* (K + \lambda I)^{-1} y$ is feasible

Define the kernel function $\kappa (x_s, x_t) = \phi (x_s)' \phi (x_t)$

The $t$th element of $k_*$ is $z'_t z'_* = \kappa (x_t, x'_*)$

The $(s, t)$th element of $K$ is $z'_s z'_t = \kappa (x_s, x_t)$
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- If we choose $\varphi$ smartly, $\kappa$ (and hence $\hat{y}_*$) will be easy to compute!
Bayesian interpretation

Like "normal" ridge regression, KRR has a Bayesian interpretation:

- **Likelihood:** $p(y|X, \beta, \theta^2) = N(Z\beta, \theta^2 I)$
- **Priors:** $p(\theta^2) \propto \theta^{-2}$, $p(\beta|\theta) = N(0, (\theta^2/\lambda) I)$
- **Posterior distribution of $y^*$** is Student's t with $T$ degrees of freedom, mode $\hat{y}^*$, variance also analytically available

Note that we can interpret $\lambda$ in terms of the signal-to-noise ratio.
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Function approximation (Hofmann, Schölkopf, Smola, 2008)
Other way to look at KRR: it also solves, for some Hilbert space $\mathcal{H}$,

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\min_{f \in \mathcal{H}} \sum_{t=1}^{T} (y_t - f(x_t))^2 + \lambda \|f\|_{\mathcal{H}}^2
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The “complexity” of the prediction function is measured by $\|f\|_{\mathcal{H}}$
Choosing the kernel function

- We can understand KRR from a Bayesian/ridge point of view, or as a function approximation technique.
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  - The prediction function $x \mapsto y$ will be linear in $\varphi(x)$, so choose a $\kappa$ that leads to a $\varphi$ for which this makes sense.
  - Complexity of the prediction function is penalized through $\| \cdot \|_H$, so choose a $\kappa$ for which this penalty ensures "smoothness."
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- We will give examples of both.
Polynomial kernel functions (Poggio, 1975)
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- Linear ridge regression: $\varphi(x) = x$ implies $\kappa(x_s, x_t) = x_s'x_t$

Interpretation of tuning parameter: higher $\sigma \Rightarrow$ smaller coefficients on higher-order terms $\Rightarrow$ smoother prediction function
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- Linear ridge regression: $\varphi(x) = x$ implies $\kappa(x_s, x_t) = x'_s x_t$
- Obvious extension: $\varphi(x) = (1, x_1, x_2, \ldots, x_1^2, x_2^2, \ldots, x_1 x_2, \ldots)'$
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- However, $\kappa$ does not take a particularly simple form in this case
- Better: $\varphi(x) = \left(1, \frac{\sqrt{2}}{\sigma}x_1, \frac{\sqrt{2}}{\sigma}x_2, \ldots, \frac{1}{\sigma^2}x_1^2, \frac{1}{\sigma^2}x_2^2, \ldots, \frac{\sqrt{2}}{\sigma^2}x_1x_2, \ldots\right)'$, which implies $\kappa(x_s, x_t) = \left(1 + \frac{x_s'x_t}{\sigma^2}\right)^2$
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- More generally, \( \kappa(x_s, x_t) = \left(1 + \frac{x_s' x_t}{\sigma^2}\right)^d \) corresponds to \( \varphi(x) = (\text{all monomials in } x \text{ up to degree } d) \)
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- Examine the effects of \( \|f\|_H \) on \( \tilde{f} \), the Fourier transform of the prediction function. Popular choice: set the kernel \( \kappa \) such that

\[
\|f\|_H \propto \int_{\mathbb{R}^N} \frac{\left|\tilde{f}(\omega)\right|^2}{\sigma^N \exp \left(-\frac{1}{2} \sigma^2 \omega' \omega\right)} d\omega
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- As $\sigma \uparrow$, components at high frequencies $\omega$ are penalized more heavily, leading to a smoother $f$
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- As $\sigma \uparrow$, components at high frequencies $\omega$ are penalized more heavily, leading to a smoother $f$

- Corresponding kernel is $\kappa(x_s, x_t) = \exp \left(\frac{-1}{2\sigma^2} \|x_s - x_t\|^2\right)$
The Gaussian kernel function (Broomhead and Lowe, 1988)

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- For a ridge regression interpretation, we would need to build infinitely many regressors of the form $\exp \left( -\frac{x'x}{2\sigma^2} \right) \prod_{n=1}^{N} \frac{x_n^{d_n}}{\sigma^{d_n} \sqrt{d_n!}}$, for nonnegative integers $d_1, d_2, \ldots, d_N$. Thus, the kernel trick allows us to implicitly work with an infinite number of regressors.
Tuning parameters

Several tuning parameters:

- Penalty parameter $\lambda$
- Smoothness parameter $\sigma$
- In our application: lag lengths (for $y$ and $X$)

Leave-one-out cross-validation can be implemented in a computationally efficient way (Cawley and Talbot, 2008)

A small (5 $\times$ 5) grid of "reasonable" values for $\lambda$ and $\sigma$ is proposed in a companion paper (Exterkate, February 2012)
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We show that replacing $\hat{y}^* = k'\left(K + \lambda I\right)^{-1}y$ by $\hat{y}^* = (k^*w^*)'(K + \lambda I W W'0)^{-1}(y_0)$ solves this problem.

Computationally efficient leave-one-out cross-validation still works.
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Time-series models

So far, we have considered $y_t = f(x_t) + u_t$

What if $x_t$ includes $y_{t-1}, \ldots, y_{t-p+1}$?

Recall Bayesian interpretation and write $p(y) = p(y_1, \ldots, y_p) \cdot p(y_{p+1} | y_p, \ldots, y_1) \cdot \ldots \cdot p(y_T | y_{T-1}, \ldots, y_1)$

Nothing changes, provided that we condition on initial values

Even stationarity does not seem to be an issue

What if $y_t$ is multivariate?

No problem whatsoever, whether or not $E_{t-1}[u_t^2]$ is diagonal

So, we could treat e.g. nonlinear VAR-like models

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In the paper: simulation study for linear and nonlinear factor models

We compare kernel ridge regression to:

- **PC**: regression of $y$ on the principal components (PCs) of $X$
- **PC$^2$$**: regression of $y$ on the PCs of $X$ and the squares of these PCs (Bai and Ng, 2008)
- **SPC**: regression of $y$ on the PCs of $(XX^T)^{1/2}$ (Bai and Ng, 2008)

Main findings:

- Kernels perform competitively for "standard" DGPs, and better for nonstandard DGPs
- Gaussian kernel is a "catch-all" method: never performs poorly; performs very well for "difficult" DGPs

Peter Exterkate (CREATES, Aarhus University)

Nonlinear Forecasting with Many Predictors using Kernel Ridge Regression
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- In the companion paper: simulation study for wide range of models, to study the effects of choosing “wrong” kernel or tuning parameters.
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- In the companion paper: simulation study for wide range of models, to study the effects of choosing “wrong” kernel or tuning parameters

- Main findings:
  - Rules of thumb for selecting tuning parameters work well
  - Gaussian kernel acts as a “catch-all” method again, moreso than polynomial kernels
Data

132 U.S. macroeconomic variables, 1959:1-2010:1, monthly observations, transformed to stationarity (Stock and Watson, 2002)

We forecast four key series: Industrial Production, Personal Income, Manufacturing & Trade Sales, and Employment

\[ y_{t+h} = 1200 \ln \left( \frac{y_{t+h}}{y_t} \right), \text{ for } h = 1, 3, 6, 12 \]

Rolling estimation window of length 120 months

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Competing models

Standard benchmarks: mean, random walk, AR

DI-AR-Lag framework (Stock and Watson, 2002): regressors are lagged $y_t$ and lagged factors

Factors extracted using PC, PC$^2$, or SPC

Lag lengths and number of factors reselected for each forecast by minimizing BIC

Kernel ridge regression: same setup, but with lagged factors replaced by $\varphi(\text{lagged } x_t)$

Polynomial kernels of degree 1 and 2, and the Gaussian kernel

Lag lengths, $\lambda$ and $\sigma$ selected by leave-one-out cross-validation
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### MSPEs for Industrial Production and Personal Income

<table>
<thead>
<tr>
<th>Forecast method</th>
<th>Industrial Production</th>
<th>Personal Income</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>h = 1</td>
<td>h = 3</td>
</tr>
<tr>
<td>Mean</td>
<td>1.02</td>
<td>1.05</td>
</tr>
<tr>
<td>RW</td>
<td>1.27</td>
<td>1.08</td>
</tr>
<tr>
<td>AR</td>
<td>0.93</td>
<td>0.89</td>
</tr>
<tr>
<td>PC</td>
<td>0.81</td>
<td>0.71</td>
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<tr>
<td>PC²</td>
<td>0.94</td>
<td>0.85</td>
</tr>
<tr>
<td>SPC</td>
<td>0.88</td>
<td>0.98</td>
</tr>
<tr>
<td>Poly(1)</td>
<td>0.79</td>
<td>0.73</td>
</tr>
<tr>
<td>Poly(2)</td>
<td>0.79</td>
<td>0.72</td>
</tr>
<tr>
<td>Gauss</td>
<td>0.76</td>
<td>0.66</td>
</tr>
</tbody>
</table>
MSPEs for Industrial Production and Personal Income

- Simple PC performs better than its nonlinear extensions
- Kernel methods perform even slightly better
- “Infinite-dimensional”, smooth Gaussian kernel is a safe choice
- Good results at all horizons
### MSPEs for Manufacturing & Trade Sales and Employment

<table>
<thead>
<tr>
<th>Forecast method</th>
<th>Manufacturing &amp; Trade Sales</th>
<th>Employment</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>$h = 1$</td>
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<tr>
<td>Mean</td>
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</tr>
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<td>0.87</td>
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</table>
MSPEs for Manufacturing & Trade Sales and Employment

- Small losses at all horizons

- Linear model is apparently sufficient here, but Gaussian KRR continues to yield adequate results

- Both PC and KRR work very well

- PC outperforms all other methods
A closer look at performance

So, KRR performs worse than PC only if PC performs very well.

To see if this result also holds over time, we computed mean squared prediction errors for each ten-year window separately.

All methods yield larger errors in more volatile periods.

However, smaller relative errors in more volatile periods.

KRR produces more volatile relative errors than PC.

⇒ KRR most valuable in turmoil periods, including 2008-9 crisis.
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Forecast encompassing regressions

Forecast encompassing regression:

\[ y_{t+h} = \alpha \hat{y}_{h,t} + u_{t+h} \]

Hypotheses of interest:

- \( \alpha = 0 \) and \( \alpha = 1 \)

Across all series and horizons,
- \( \alpha = 0 \) is strongly rejected for PC and for all KRR forecasts
- In many cases, \( \alpha = 1 \) cannot be rejected
- Thus, PC and KRR forecasts encompass AR forecasts
Forecast encompassing regressions

Forecast encompassing regression:

\[ y_{t+h} = \alpha \hat{y}_{t+h|t}^{PC \text{ or KRR}} + (1 - \alpha) \hat{y}_{t+h|t}^{AR} + u_{t+h} \]
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Peter Exerkate (CREATES, Aarhus University)  Nonlinear Forecasting with Many Predictors using Kernel Ridge Regression
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Also compare kernels and PC:

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▶ That is, \( 0 < \alpha < 1 \): KRR and PC forecasts are complements
Conclusions

Kernel ridge regression provides a natural way of dealing with high-dimensionality and nonlinearity. It can also handle time-series models with constant conditional volatilities and correlations, even if they are nonstationary. Selection of kernel and tuning parameters can be fully automated: easy-to-use black-box implementation for nonlinear forecasting. Macro forecasting: KRR outperforms more traditional methods. Best forecast performance in turmoil periods. The "smooth" Gaussian kernel generally performs best.
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- The “smooth” Gaussian kernel generally performs best.
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- So far, Gaussian kernel holds up very well
- Extend the methodology to models with time-varying volatility
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